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# Lecture Series in Computational Fluid Dynamics

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Kevin W. Thompson

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Kevin W. Thompson, Ames Research Center, Moffett Field, California

August 1987



National Aeronautics and  
Space Administration

**Ames Research Center**  
Moffett Field, California 94035



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# Introduction

This text was written to accompany a series of lectures on computational methods for fluid dynamics problems, which I gave in the Space Science Division at NASA Ames Research Center in July and August of 1986. Each chapter in the text corresponds to a particular lecture. Sufficient interest was expressed in the subject that Lynda Haines, the User Services Manager of the Numerical Aerodynamic Simulator (NAS) Project, asked me to prepare a series of videotaped lectures to be distributed along with this text. Anyone interested in obtaining these tapes should contact NAS User Services at NASA Ames Research Center, Moffett Field, CA 94035.

This lecture series covers the basic principles of computational fluid dynamics (abbreviated as "CFD" throughout). The lectures are designed to teach an inexperienced person everything he or she needs to know to create a time dependent numerical model of fluid flow, in one or more dimensions. I say "a model" because there is no unique way to construct numerical models, and the number of such models which have been constructed greatly exceeds the number of practitioners in the field.

As there are so many different approaches to simulating fluid flow, it is appropriate to consider what will and will not be covered by these lectures. Lagrangian methods, in which the computational grid moves with the fluid, will not be covered at all. Time implicit methods will be mentioned, but not described in detail. Accelerated convergence to steady states and boundary stability theory will be ignored. Finally, the great majority of time explicit schemes, clever or otherwise, cannot be examined due to lack of time, especially as some of them are quite complicated. This is not a survey course in computational methods.

What will be covered are the basic concepts fundamental to every CFD scheme. The emphasis will be on concepts and techniques which are simple, general, and have a clear mathematical basis (criteria which exclude a great many methods in use!). While the mathematical underpinnings are important, the usability of the methods is equally important; therefore mathematical rigor will not be attempted, as the focus will be on the concepts rather than their proof. Indeed, mathematically rigorous statements can seldom be made about solution methods for CFD problems. Virtually all rigorous mathematical work has been devoted to the simpler problems of linear systems or single nonlinear equations. Fortunately, techniques developed for these simpler problems usually work on the more complicated problems of nonlinear systems, even in the absence of mathematical proofs that they should do so.

One standard of maturity for a field is the degree to which all conclusions follow logically from a small number of basic principles. By this standard, computational

fluid dynamics is not a mature field. It has been characterized by a large collection of complicated *ad hoc* methods. These lectures will try to achieve some maturity by getting a widely applicable approach from a small number of basic concepts. In this sense it departs from the "traditional" path in the CFD field, which has been to get the best possible solutions to specialized problems.

*Acknowledgment.* I have performed this work while a National Research Council Research Associate, doing research into astrophysics in the Space Science Division at NASA Ames Research Center. I am indebted to the NRC, NASA Ames, and the Space Science Division for supporting me in this work. I would also like to express my appreciation to the NAS Project for sponsoring the production of the videotapes.

# Chapter 1

## Conservation Laws, Wave Equations, and Shocks

This chapter deals with the general properties of hyperbolic systems of conservation laws, of which the most frequently encountered example is probably the fluid dynamics equations. It begins by defining what one means by “conservation,” and describes the close relationship between conservation laws and wave equations. We quickly discover that the concept of a continuous function as the solution of a partial differential equation is inadequate when we consider nonlinear equations, and are thus led to the concept of *shock waves* as the required discontinuous solutions. We will also find that not all shock waves which are allowed by conservation arguments are physically valid solutions, and that only those shocks which satisfy an *entropy condition* may actually occur.

### 1.1 Conservation Laws

The equations of fluid dynamics are one example of the mathematical formulation of conservation laws. The simplest one dimensional conservation law is a single equation, describing a single conserved quantity, and may be written as either an integral equation or as a partial differential equation. Suppose (in one dimension) that  $u$  is the density of some conserved quantity per unit length, and  $f$  is the flux of  $u$  (i.e., the rate at which the density  $u$  flows past a given  $x$  coordinate). The integrated density between two points  $x_1$  and  $x_2$ ,  $x_2 < x_1$ , satisfies [1]

$$\frac{d}{dt} \int_{x_2}^{x_1} u(x, t) dx = -[f(x_1, t) - f(x_2, t)]. \quad (1.1)$$

If  $u$  and  $f$  are continuous functions of  $x$  and  $t$ , then in the limit as  $x_2 \rightarrow x_1 \equiv x$ , Eq. (1.1) becomes

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0. \quad (1.2)$$

Eq. (1.2) is said to be in *conservation form*. More generally, any equation in which the time derivative of a density plus the divergence of a flux equals inhomogeneous local

(i.e., non-derivative) source terms is in conservation form. In the case of (1.2), the flux divergence is  $\partial f / \partial x$ , and the source terms are zero.

The conservation form of an equation or system relates the time rate of change of a density in a small volume to the flux of that quantity through the boundary of that volume. Alternatively, one may recast the problem in terms of waves, and study the propagation of wave amplitudes. The two approaches are nearly the same when applied to single linear equations; however they are quite different, though still related, when applied to nonlinear systems such as the fluid dynamics equations. The equivalent wave equations are usually called *characteristic equations* in this context, while the wave velocities are called *characteristic velocities*.

## 1.2 Wave Equations

We begin by introducing the wave amplitude  $u$ , which is a function of the time  $t$  and the spatial coordinate  $x$ . Suppose there exists a curve  $C$  in the  $xt$  plane, parameterized by the variable  $\sigma$  through the relations

$$x = x(\sigma), \quad t = t(\sigma), \quad (1.3)$$

where each point on  $C$  corresponds to a unique value of  $\sigma$ . Then the rate of change of  $u$  along the curve  $C$  is [2]

$$\frac{du}{d\sigma} = \frac{\partial u}{\partial t} t_\sigma + \frac{\partial u}{\partial x} x_\sigma, \quad (1.4)$$

where the subscripts denote derivatives with respect to  $\sigma$ .

If  $u(x, t)$  is constant along  $C$ , we have

$$\frac{du}{d\sigma} = 0, \quad (1.5)$$

and  $C$  is called the *characteristic curve*, or simply *characteristic*, of  $u$ . Eq. (1.5) is called a characteristic equation, and may be cast in different forms.

A common form for the characteristic equation is obtained by dividing (1.4) (with  $du/d\sigma = 0$ ) by  $t_\sigma$  (implicitly assuming that  $t_\sigma$  is never zero; we will assume that  $t(\sigma)$  is always an increasing function of  $\sigma$ , as in  $t = \sigma$ ), giving

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0, \quad a = x_\sigma / t_\sigma = dx/dt, \quad (1.6)$$

where  $a$  is the characteristic (or wave) velocity and is simply the slope of curve  $C$  in the  $xt$  plane. If  $a$  is constant, Eq. (1.6) is a linear wave equation. If  $a = a(u) \neq \text{constant}$ , Eq. (1.6) is a nonlinear wave equation.

The conservation and wave equations for  $u$  are equivalent provided that the wave speed  $a$  is given by

$$a = \frac{df}{du}. \quad (1.7)$$

If  $a = \text{constant}$ , the problem is linear and the solution is

$$u(x, t) = u_0(x - at), \quad \text{where } u(x, 0) = u_0(x). \quad (1.8)$$

The characteristics in the linear case are a family of parallel lines with constant slope  $dx/dt = a$ , along each of which  $u = \text{constant}$ , although  $u$  varies from one line to the next. The characteristics cover the entire  $xt$  plane in the region  $t \geq 0$ , implying that the solution exists as defined for all  $x$  and  $t \geq 0$ .

The derivative  $du/d\sigma$  on the left side of (1.4) is often written with  $\sigma \equiv t$ , as in

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + \frac{dx}{dt} \frac{\partial u}{\partial x}, \quad (1.9)$$

in which case it is called the total time derivative. The quantity  $du/dt$  in Eq. (1.9) represents the time rate of change of  $u$  as measured at a point moving with velocity  $dx/dt$ .

### 1.3 Continuous Analytical Solutions

Now consider the general case where  $a(u)$  is not constant. We know that  $u$  is constant along each characteristic curve  $C$  in the  $xt$  plane, hence  $a(u)$  is also constant and the characteristics are straight lines. However, as  $u$  varies from one characteristic to the next, so does  $a(u)$ , and the slopes of the characteristics also vary from one to the next. Those characteristics which are initially separate will either diverge or converge, leading to behavior not seen in the linear problem. A typical characteristic diagram is shown in Figure 1.1, reproduced from page 21 of the book by Whitham [1].

Let the initial value problem be given by Eq. (1.6) with  $u(x, 0) = f(x)$ . Then for each characteristic curve which intersects the  $x$  axis at  $x = \xi$  at time  $t = 0$ ,  $u = f(\xi)$  everywhere on that curve. The slope of a given curve is  $a(f(\xi)) \equiv F(\xi)$  and is also known. Each characteristic is therefore defined by a unique  $\xi$  value, and has as its equation

$$x = \xi + F(\xi)t. \quad (1.10)$$

The complete set of  $\xi$  values defines a whole family of characteristics, along each of which the solution is

$$u = f(\xi), \quad a = F(\xi) = a(f(\xi)). \quad (1.11)$$

Now let's check the solution. We find

$$\frac{\partial \xi}{\partial x} = \frac{1}{1 + F'(\xi)t}, \quad \frac{\partial \xi}{\partial t} = -\frac{F(\xi)}{1 + F'(\xi)t}, \quad (1.12)$$

where the primes denote derivatives with respect to  $\xi$ , and therefore

$$\frac{\partial u}{\partial t} = -\frac{F(\xi)f'(\xi)}{1 + F'(\xi)t}, \quad \frac{\partial u}{\partial x} = \frac{f'(\xi)}{1 + F'(\xi)t}, \quad (1.13)$$

and Eq. (1.6) is satisfied.

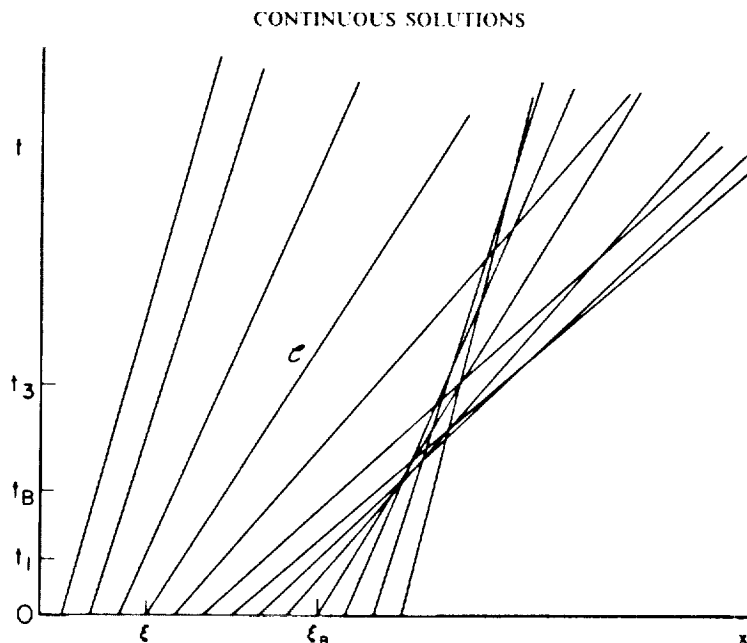


Figure 1.1: Characteristic Diagram for Nonlinear Waves. Copyright © 1974 by John Wiley & Sons, Inc. Reprinted by permission of John Wiley & Sons, Inc.

Saying that  $u$  is constant along a characteristic curve whose slope is  $a(u) = dx/dt$  is equivalent to saying that each particular value of  $u$  propagates at a characteristic velocity  $a(u)$ , which is the wavelike behavior we were seeking. In the linear case where  $a(u) = \text{constant}$ , the solution obtained above reduces to the simple form of Eq. (1.8). In the nonlinear case, the velocity changes from point to point and the wave exhibits a nonlinear distortion.

## 1.4 The Breaking of Waves

Difficulties arise when the wave undergoes compression, which occurs in any region where the velocity  $a$  is decreasing, i.e., in any region for which  $F'(\xi) < 0$ . Any two characteristics in this region which are initially separate will cross at some later time, giving a solution which is multivalued. This difficulty is apparent in the solution of (1.13): the wave “breaks” (acquires an infinite slope) at the time  $t = -1/F'(\xi)$ . Breaking occurs earliest on the characteristic defined by  $\xi = \xi_B$  for which  $F'(\xi) < 0$  and  $|F'(\xi)|$  is the maximum, and at a time  $t_B$  given by

$$t_B = -\frac{1}{F'(\xi_B)}. \quad (1.14)$$

An extreme case of breaking occurs when the initial state is a step function at  $x = 0$ ,

with

$$u(x, 0) = f(x) = \begin{cases} u_1, \\ u_2, \end{cases} \quad a(x, 0) = F(x) = \begin{cases} a_1 = a(u_1), & x > 0, \\ a_2 = a(u_2), & x < 0. \end{cases} \quad (1.15)$$

If  $a_2 > a_1$  the solution breaks immediately.

A different result occurs if  $a_2 < a_1$ . The wave undergoes expansion, and a continuous solution results. At times  $t > 0$  all values of  $F(0)$  between  $a_1$  and  $a_2$  spread out along a fan of characteristics passing through  $\xi = 0$ . This *expansion fan* is continuous, and must satisfy (1.10) and (1.11), hence

$$a = \frac{x}{t}, \quad a_2 < \frac{x}{t} < a_1, \quad (1.16)$$

and the complete solution for  $a$  is

$$a = \begin{cases} a_1, & a_1 < x/t; \\ x/t, & a_2 < x/t < a_1; \\ a_2, & x/t < a_2. \end{cases} \quad (1.17)$$

The solution for  $u(x, t)$  is then obtained by inverting the known relationship  $a = a(u)$ .

## 1.5 Shock Waves

In practice, the nonlinear wave equation we wish to solve represents a process whose physical reality must be single valued, and the multi-valued solution produced by wave breaking must be rejected. Yet solution (1.10)–(1.13) is valid up until the derivatives become infinite, so we must modify our concept of a solution to include discontinuous solutions which are single valued, and have a finite number of discontinuities. The formulation of the wave problem as a partial differential equation is not valid for discontinuous solutions, because the derivatives are defined only for continuous functions. However, the *integral* formulation of conservation law (1.1) is valid even when  $u$  is discontinuous, and it is to this form we turn now.

Stable discontinuities in nonlinear waves are called shock waves, or shocks. On either side of the shock the solution is continuous and differentiable. If the shock is located at position  $x_s(t)$  and moves with velocity  $v_s$ , where  $x_2 < x_s(t) < x_1$  at time  $t$ , we may write the integral equation for  $u$  as [1]

$$f(x_2, t) - f(x_1, t) = \frac{d}{dt} \int_{x_2}^{x_s^-} u(x, t) dx + \frac{d}{dt} \int_{x_s^+}^{x_1} u(x, t) dx, \quad (1.18)$$

$$= \int_{x_2}^{x_s^-} \frac{\partial}{\partial t} u(x, t) dx + u(x_s^-, t) v_s + \int_{x_s^+}^{x_1} \frac{\partial}{\partial t} u(x, t) dx - u(x_s^+, t) v_s. \quad (1.19)$$

In the limit as  $x_2 \rightarrow x_s^-$ ,  $x_1 \rightarrow x_s^+$  this becomes the *shock jump condition*

$$f_2 - f_1 = v_s(u_2 - u_1), \quad (1.20)$$

where  $f_1$ ,  $u_1$  are the flux and value of  $u$  on side 1 of the shock (taken to be the right here), and  $f_2$ ,  $u_2$  are the values on side 2.

The shock jump condition may also be obtained by transforming the conservation equation (1.2) to a reference frame in which the shock is at rest; i.e., which moves at a velocity  $v_s$  with respect to the original coordinate system. Integrating the transformed equation over a small volume around the shock, and taking the limit as the volume goes to zero, shows that the transformed flux  $f - uv_s$  must be continuous across the shock. Thus  $f_1 - u_1v_s = f_2 - u_2v_s$ , which gives Eq. (1.20).

Rewriting (1.20) gives the shock velocity as

$$v_s = \frac{f(u_2) - f(u_1)}{u_2 - u_1}. \quad (1.21)$$

In the weak shock limit where  $|u_2 - u_1| \ll |u_2| + |u_1|$  we have  $u_2 \approx u_1 = u$ , and  $v_s \rightarrow \partial f / \partial u \equiv a(u)$ . Thus a sufficiently weak shock is a small discontinuity which travels at the local wave velocity. A strong shock, however, has a velocity which is distinct from both  $u_1$  and  $u_2$ . Note that  $v_s = a$  always for the linear wave equation, where  $a = \text{constant}$ .

## 1.6 The Inviscid Burger's Equation

Perhaps the most well known nonlinear wave equation is the inviscid Burger's equation

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0, \quad \text{or} \quad \frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left( \frac{u^2}{2} \right) = 0, \quad (1.22)$$

which has  $f(u) = u^2/2$ ,  $a(u) = u$ . Burger's equation appears in most texts on nonlinear hyperbolic equations, and in the inviscid form represents the velocity field of a gas of non-interacting particles (such as a cloud of dust particles in a vacuum, or a zero pressure gas).

The inviscid Burger's equation satisfies the general solutions obtained above. Its solution for an initial discontinuity at  $x = 0$ , with  $u = u_2$  at  $x < 0$ ,  $u = u_1$  at  $x > 0$ , is an expansion fan for  $u_2 < u_1$ :

$$u(x, t) = \begin{cases} u_2, & x/t < u_2; \\ x/t, & u_2 < x/t < u_1; \\ u_1, & u_1 < x/t; \end{cases} \quad (1.23)$$

and a shock wave for  $u_2 > u_1$ :

$$u(x, t) = \begin{cases} u_2, & x < v_s t; \\ u_1, & x > v_s t; \end{cases} \quad (1.24)$$



where the shock velocity is obtained from (1.21):

$$v_s = \frac{1}{2}(u_2 + u_1). \quad (1.25)$$

The linear wave equation and the nonlinear Burger's equation represent special cases of one dimensional planar fluid flow. If the fluid velocity  $v$  is constant with  $x$ , then the continuity equation for the density reduces to (1.6), with  $u$  the density and  $a = v =$  constant the fluid velocity. Density inhomogeneities are carried along by the flow without distortion. However, if the pressure is *spatially* constant ( $\partial p / \partial x = 0$ ), then the velocity equation reduces to the inviscid Burger's equation, with  $u$  the fluid velocity.

## 1.7 Expansion Shocks and the Entropy Condition

The preceding analysis found two different solutions to the nonlinear wave problem with a step function initial condition. The case with  $a_2 > a_1$  remains a step function, the discontinuity being a shock wave which propagates at the shock velocity given by Eq. (1.21). The case with  $a_2 < a_1$  breaks up into an expansion fan (which widens with time) adjoining the constant states  $u_2$  and  $u_1$  on either side.

The shock jump condition (1.20) says nothing about the breakup of a discontinuity into an expansion fan. It is natural to ask if a discontinuity between two states with  $a_2 < a_1$  could also propagate as a shock, since the possibility is permitted by the jump condition. Such a shock is known as an *expansion shock*, since it leaves behind a state of decreased "density"  $u$ .

It turns out that expansion shocks are unstable. Small perturbations to an expansion shock solution grow, destroying the shock. Compression shocks, on the other hand, are stable. Stable shocks must satisfy the *entropy condition* [1], [3]

$$a_2 > v_s > a_1, \quad (1.26)$$

which means that characteristics cross at the shock front, and the slope of the shock front line in the  $xt$  plane lies between the slopes of the characteristics which intersect it from either side. Consequently no characteristic drawn in the direction of decreasing  $t$  intersects a line of discontinuity, and every point in the plane can be connected by a backward drawn characteristic to a point on the initial line at  $t = 0$ . In the case of the inviscid Burger's equation,  $a = u$ , and  $v_s = (u_2 + u_1)/2$ , which satisfies (1.26) only for  $u_2 > u_1$ , as expected.

Expansion shocks are forbidden solutions for systems of nonlinear equations as well. In the case of fluid dynamics, an expansion shock would cause the entropy of the flow to decrease with time, and is forbidden by the laws of thermodynamics as well as stability considerations. It is for this reason that criteria such as (1.26) are known as entropy conditions.

## 1.8 Nonlinear Systems in One Dimension

In this section we consider systems of conservation laws of the form

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} = 0, \quad \mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ \dots \\ u_n \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} f_1 \\ f_2 \\ \dots \\ f_n \end{pmatrix}. \quad (1.27)$$

where  $\mathbf{f}$  is a vector flux and a function of the conserved densities which are the components of the vector  $\mathbf{u}$ . (Note that the term vector is used here in the linear algebra sense to represent any set of unknowns, and not, for example, as a velocity vector.)

As in the previous section, let the states on either side of a shock be numbered 1 and 2 (1 for the right side, 2 for the left). The shock jump conditions are obtained by writing Eq. (1.27) in integral form, and integrating over a small region containing the shock, as in section 1.5. The  $n$  jump conditions are therefore

$$f_{i2} - f_{i1} = v_s(u_{i2} - u_{i1}), \quad i = 1, \dots, n, \quad (1.28)$$

where  $f_{i1} = f_i(\mathbf{u}_1)$  is the  $i$ th flux on side 1 of the shock, and similarly for  $f_{i2}$ . The shock velocity  $v_s$  is the same for all  $n$  jump conditions.

Eq. (1.27) can also be written in the form

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{u}}{\partial x} = 0, \quad \text{or} \quad \frac{\partial u_i}{\partial t} + \sum_{j=1}^n a_{ij} \frac{\partial u_j}{\partial x} = 0, \quad i = 1, \dots, n, \quad (1.29)$$

where  $\mathbf{A}$  is the Jacobian matrix of elements  $a_{ij}$  defined by

$$a_{ij} = \frac{\partial f_i}{\partial u_j}. \quad (1.30)$$

The system is defined to be hyperbolic if the matrix  $\mathbf{A}$  has  $n$  real eigenvalues  $\lambda_i$ , which we will order so that  $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ . The eigenvalues are the characteristic velocities at which signals propagate in the medium described by (1.27). The characteristic velocities are the slopes of the characteristic curves, as was the case for the single wave equation. However, constancy of any wave amplitude along a characteristic curve no longer implies constancy of the wave velocity along that curve, so the characteristic curves need no longer be straight, and in general will not be. (A more detailed discussion of the characteristic equations for nonlinear systems will be given in Chapter 5.)

The characteristic velocities determine an entropy condition for the nonlinear system, which defines the class of allowed shock waves in a fashion analogous to Eq. (1.26). The entropy condition for the nonlinear system, as given by Lax [3], is that for some value of  $k$ ,  $1 \leq k \leq n$ , the inequality

$$\lambda_k(\mathbf{u}_2) > v_s > \lambda_k(\mathbf{u}_1) \quad (1.31)$$

must be satisfied.

In the case of fluid dynamics, the characteristic velocities are  $\lambda_1 = v - c$ ,  $\lambda_2 = v$ , and  $\lambda_3 = v + c$ , where  $v$  is the fluid velocity and  $c$  is the speed of sound. If the shock speed is positive, Eq. (1.31) is satisfied by the case  $k = 3$ :

$$v_2 + c_2 > v_s > v_1 + c_1, \quad (v_s > 0), \quad (1.32)$$

which means that right-moving sound waves on either side of the shock intersect the shock. If the shock speed is negative, then

$$v_2 - c_2 > v_s > v_1 - c_1, \quad (v_s < 0), \quad (1.33)$$

which is the  $k = 1$  condition, and implies that all left-moving sound waves intersect the shock.

In either case, sound waves behind the shock (in the compressed region) travel faster than the shock and catch up to it, while sound waves in front of the shock are propagating more slowly than the shock and are overtaken by it. Thus the shock velocity is subsonic relative to the post-shock state, but supersonic relative to the pre-shock state. Very weak shock waves (characterized by very small shock jumps) are simply sound waves, and travel at the speed of sound relative to the fluid. In this limit, the three velocities in (1.32) become the same.

## 1.9 Exercises

1. Verify that the solution of (1.10)–(1.11) satisfies the integral equation (1.1), for the linear case where  $F(\xi) = a = \text{constant}$ .
2. Find the shock jump condition for the equation

$$\frac{\partial}{\partial t} \left( \frac{1}{2} u^2 \right) + \frac{\partial}{\partial x} \left( \frac{1}{3} u^3 \right) = 0.$$

Is it the same as (1.25) for Burger's equation? Does this result seem unusual?

*Comment:* A particular conservation law, such as (1.22), will give rise to an infinite number of other equations upon multiplication by  $u$  to some power. The resulting equations are equivalent for  $u$  a continuous function, but give rise to different shock jump conditions. The correct jump condition may only be determined by reference to the physics of the problem, i.e., by working with those quantities which are both conserved and physically meaningful, such as mass, momentum, and energy.

3. The general expansion fan  $u = (x - x_0)/(t - t_0)$  is a solution to the inviscid Burger's equation (1.22). Consider an initial value problem given by  $u = x/(1+t)$  for  $x < x_0$ ,  $u = 0$  for  $x > x_0$ , at time  $t = 0$ . The point  $x_0$  is the initial shock location. Find the solution for  $t > 0$ , including the shock location  $x_s$  and shock velocity  $v_s$ . (*Hint:*  $v_s$  is not constant with time.)

4. The fluid equations for a perfect gas in one dimension are

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) &= 0, \\ \frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho v^2 + p) &= 0, \\ \frac{\partial}{\partial t} \left( \frac{1}{2} \rho v^2 + e \right) + \frac{\partial}{\partial x} \left[ \left( \frac{1}{2} \rho v^2 + e + p \right) v \right] &= 0,\end{aligned}$$

where  $\rho$  is the mass density,  $v$  is the velocity,  $p = (\gamma - 1)e$  is the pressure,  $e$  is the thermal energy density, and  $\gamma$  is the (constant) ratio of specific heats ( $= 5/3$  for an atomic gas). Find the shock jump conditions. Show that

$$\frac{\rho_2}{\rho_1} = \frac{(\gamma + 1)p_2/p_1 + (\gamma - 1)}{(\gamma - 1)p_2/p_1 + (\gamma + 1)}.$$

If  $p_2/p_1$  can range from one to infinity, what values can the density ratio  $\rho_2/\rho_1$  take on? (*Hint*: Although there are now three shock jump conditions, there is still only one shock velocity.)

5. Using the shock jump conditions derived in the previous problem, let  $\rho_1 = p_1 = 1$ ,  $v_1 = 0$ ,  $\gamma = 5/3$ , and  $p_2/p_1 = 5$ . The speed of sound is  $c = \sqrt{\gamma p/\rho}$ . Compute  $\rho_2$ ,  $v_2$ , and  $v_s$ , draw a diagram of the pre- and post-shock characteristics, and show that condition (1.32) is satisfied.

Condition (1.32) is condition (1.31) with  $k = 3$ . For this problem, is condition (1.31) satisfied for any other  $k$ ?

## Chapter 2

# Finite Difference Solutions of Wave Equations

The first chapter considered the general properties of conservation laws and wave equations in one dimension. This chapter will cover the basic concepts involved in the approximate solution of wave equations by finite difference methods. The conservation laws of interest are partial differential equations in one time and one or more spatial coordinates.

The numerical techniques to be described in this chapter will be oriented at first toward the solution of the linear wave equation, in order to introduce the basic concepts without obscuring them by the complexity encountered in solving nonlinear systems. However, since the solution of nonlinear systems in more than one spatial dimension is our ultimate goal, the implications of nonlinear systems for the solution techniques presented will be discussed after each technique is described. In Chapter 4 we will find that consideration of the very general problem of multidimensional nonlinear systems with shocks will determine the form of an artificial viscosity. This chapter will demonstrate the need for artificial viscosity in problems with discontinuous solutions and will introduce a form suited for the problems under discussion, but the fundamental justification of the form will be deferred to Chapter 4.

### 2.1 Basic Finite Difference Approximations

We begin by considering a piecewise continuous function  $f(x)$ , defined for all  $x$ . Ideally, we would like to know the exact value of  $f$  for all  $x$  values, but in practice we will be restricted to knowing  $f$  at a finite number of discrete points. Describing a function in terms of its values at discrete points is known as *discretization*. For convenience sake, we will discretize  $f(x)$  by recording its values at the set of grid points  $x_i$ , spaced a uniform distance  $\Delta x$  apart,

$$x_i = i\Delta x, \quad (2.1)$$

although in general one can have arbitrary grid spacing, which leads to more complicated finite difference approximations. Denote the values of  $f$  at  $x_i$  by  $f_i$ :

$$f_i = f(x_i). \quad (2.2)$$

Given the  $f_i$  values, we need to approximate various derivatives of  $f$  at the grid points. The starting point for all such approximations is the discrete Taylor's series [4],

$$f_{i+n} = f_i + n\Delta x \left. \frac{df}{dx} \right|_i + \frac{(n\Delta x)^2}{2!} \left. \frac{d^2 f}{dx^2} \right|_i + \cdots + \frac{(n\Delta x)^m}{m!} \left. \frac{d^m f}{dx^m} \right|_i + \cdots, \quad (2.3)$$

which holds for  $f(x)$  a continuous and infinitely differentiable function. If  $f(x)$  is not continuous, this approximation breaks down and difficulties may occur. Techniques for dealing with discontinuous functions will be discussed later. For now we will assume that all functions are continuous.

Setting  $n = \pm 1$ , we see immediately that

$$\left. \frac{df}{dx} \right|_i = \frac{1}{\Delta x} (f_{i+1} - f_i) + O(\Delta x), \quad (2.4)$$

$$= \frac{1}{\Delta x} (f_i - f_{i-1}) + O(\Delta x). \quad (2.5)$$

Eqs. (2.4) and (2.5) are called one sided difference approximations, and are the basis for the low order upwind schemes to be discussed later. These one sided formulas are formally of first order accuracy. The order of an approximation is given by the power of the grid spacing  $\Delta x$  appearing in the leading error term, since the error in the approximation vanishes as that power of  $\Delta x$  in the limit as  $\Delta x \rightarrow 0$ . We can see that the one sided approximations are first order accurate by solving for  $df/dx|_i$  in Eq. (2.3) with  $n = 1$ :

$$\left. \frac{df}{dx} \right|_i = \frac{1}{\Delta x} (f_{i+1} - f_i) - \frac{\Delta x}{2!} \left. \frac{d^2 f}{dx^2} \right|_i - \frac{(\Delta x)^2}{3!} \left. \frac{d^3 f}{dx^3} \right|_i - \cdots - \frac{(\Delta x)^{m-1}}{m!} \left. \frac{d^m f}{dx^m} \right|_i - \cdots. \quad (2.6)$$

For a sufficiently small  $\Delta x$ , the leading error term dominates, hence Eq. (2.4) is a first order approximation to  $df/dx|_i$ , as is Eq. (2.5).

The first order approximations are useful in certain situations (such as at a boundary, where symmetrically located data are not available), but their slow convergence properties make them undesirable in most instances if more accurate approximations are available.

Replacing  $n$  by  $\pm n$  in Eq. (2.3) and taking the difference of the expressions yields the following result:

$$T_n^2 \equiv \frac{f_{i+n} - f_{i-n}}{2n\Delta x} = \left. \frac{df}{dx} \right|_i + \frac{(n\Delta x)^2}{3!} \left. \frac{d^3 f}{dx^3} \right|_i + \frac{(n\Delta x)^4}{5!} \left. \frac{d^5 f}{dx^5} \right|_i + \frac{(n\Delta x)^6}{7!} \left. \frac{d^7 f}{dx^7} \right|_i + \cdots, \quad (2.7)$$

from which we get the second order approximation

$$\left. \frac{df}{dx} \right|_i = \frac{f_{i+1} - f_{i-1}}{2\Delta x} + O(\Delta x^2). \quad (2.8)$$

Note that Eq. (2.8) is not the only centered second order approximation. The quantity  $T_n^2$ , defined by Eq. (2.7), is a second order approximation to  $df/dx|_i$  for any  $n$  value. However, the error is quadratic in  $n$ , so the case  $n = 1$  is clearly the best choice.

We've seen first and second order approximations to  $df/dx$ . Higher order approximations may be constructed by taking appropriate linear combinations of the formulas already obtained. For example, Eq. (2.7) gives an exact expression for the error terms in the approximation  $T_n^2$ . The following linear combination gives a fourth order approximation to  $df/dx|_i$ :

$$T_n^4 \equiv \frac{n^2 T_1^2 - T_n^2}{n^2 - 1} = \frac{df}{dx}\bigg|_i - \frac{n^4 - n^2}{n^2 - 1} \frac{\Delta x^4}{5!} \frac{d^5 f}{dx^5}\bigg|_i - \frac{n^6 - n^2}{n^2 - 1} \frac{\Delta x^6}{7!} \frac{d^7 f}{dx^7}\bigg|_i - \dots \quad (2.9)$$

The leading error term is again quadratic in  $n$ , and is minimized for  $n = 2$  (note that  $n$  may not be 1), giving

$$T_2^4 = \frac{4}{3} T_1^2 - \frac{1}{3} T_2^2 \quad (2.10)$$

as the best fourth order approximation to  $df/dx|_i$ :

$$\frac{df}{dx}\bigg|_i = \frac{1}{12\Delta x} [8(f_{i+1} - f_{i-1}) - (f_{i+2} - f_{i-2})] + O(\Delta x^4). \quad (2.11)$$

Higher order approximations are obtained by computing lower order approximations over different intervals  $n\Delta x$ , then taking linear combinations of the results with coefficients chosen to cancel out the leading error term.

The above approach is an application of *Richardson extrapolation*, or the deferred approach to limit [4]. Richardson extrapolation can be used to obtain improved, higher order estimates of any quantity whose error is known to consist of a power series in some discretization parameter. One computes the lowest order approximation to the quantity using different discretization parameters (such as  $n\Delta x$  in the above example), then takes linear combinations of the two most accurate lower order approximations to obtain a higher order approximation. In the above example, only even powers of the discretization parameter appeared in the power series, so that a fourth order approximation was obtained very quickly. In other circumstances, such as the first order approximations of Eq. (2.6), all powers of the discretization parameter appear and more work is required to obtain a given order of accuracy.

Another common example of Richardson extrapolation is Romberg's method for approximating definite integrals. One computes a sequence of trapezoidal approximations to the integral, using different interval sizes, then takes linear combinations of the results to eliminate the leading error terms. The resulting approximation yields a much more accurate approximation for a given amount of effort than does the trapezoidal approximation by itself.

A similar analysis leads to the following formula for the second derivative of a function, to second order:

$$\frac{d^2 f}{dx^2}\bigg|_i = \frac{1}{\Delta x^2} (f_{i+1} - 2f_i + f_{i-1}) + O(\Delta x^2). \quad (2.12)$$

One also encounters diffusion terms, which may be approximated as

$$\frac{d}{dx} \left( \kappa \frac{df}{dx} \right) = \frac{1}{\Delta x^2} [\kappa_{i+1/2} (f_{i+1} - f_i) - \kappa_{i-1/2} (f_i - f_{i-1})] + O(\Delta x^2), \quad (2.13)$$

and which reduces to Eq. (2.12) for the case  $\kappa = 1$ .

## 2.2 A Brief Survey of "Traditional" Solution Methods

Having mastered the basics of finite difference approximations, we will now attempt to solve the one dimensional linear wave equation

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0, \quad a = \text{constant}, \quad (2.14)$$

on a grid in the  $xt$  plane, at the points  $(x_i, t^n)$ , spaced evenly in the  $x$  direction ( $x_i = i\Delta x$ ) but not necessarily in the  $t$  direction. Let  $U_i^n \equiv U(x_i, t^n)$  be the numerical approximation to the exact solution  $u(x, t)$  at the grid points.

We are given a partial differential equation which relates the time variations in a quantity  $u$  to its spatial variations, as well as initial data for all  $x$  values. The approximate solution at a time  $\Delta t$  later is obtained from a numerical approximation to the differential equation. Repeated applications of the numerical approximation yield solutions at a sequence of advancing time steps.

The solution to the problem is completely defined once we have the differential equation and the initial data; hence the problem is called an *initial value problem*. A related, but more complicated, problem is the *initial boundary value problem*, in which boundary conditions as well as initial conditions over a finite spatial domain are specified. I will return to the issue of boundary conditions in Chapter 5, but for now we will look at the finite difference solution of wave equations over an infinite domain.

The literature describing methods for solving wave equations and conservation laws is very large, and a comprehensive examination of all such methods is not feasible. Instead we will look a few representative and commonly used methods, chosen not only because they illustrate the basic concepts of numerical solutions but also because they may be applied to a wide variety of problems.

### 2.2.1 First Order Upwind Methods

The simplest and least accurate solution methods for the linear equation are the first order "upwind" methods. Replacing the time and space derivatives in Eq. (2.14) by their first order approximations yields four possible solutions:

$$U_i^{n+1} = U_i^n - \sigma(U_i^n - U_{i-1}^n), \quad (2.15)$$

$$U_i^{n+1} = U_i^n - \sigma(U_{i+1}^n - U_i^n), \quad (2.16)$$

$$U_i^{n+1} = U_i^n - \sigma(U_i^{n+1} - U_{i-1}^{n+1}), \quad (2.17)$$

$$U_i^{n+1} = U_i^n - \sigma(U_{i+1}^{n+1} - U_i^{n+1}), \quad (2.18)$$

where

$$\sigma = a \frac{\Delta t}{\Delta x} \quad (2.19)$$

is called the *Courant number*, after Richard Courant, whose work in linear and nonlinear waves and their solution forms the foundation for much of the field today.



At first glance these four approximations may seem equally valid—and they are from the standpoint of the formal accuracy of the approximations out of which they were constructed. However, two of them are guaranteed to be unstable for any time step size  $\Delta t$ . Stability analysis will be deferred to Chapter 3, but for now it will simply be stated that Eqs. (2.16) and (2.18) are unstable if  $a > 0$ , while Eqs. (2.15) and (2.17) are unstable if  $a < 0$ . "Instability" means that the numerical solution grows exponentially with the number of time steps, even though exponential growth is not a valid solution to the given initial value problem.

The stability criteria for the upwind methods illustrate a very general property of numerical solution methods, which can be stated as follows: *The domain of dependence of the numerical approximation to the solution of the differential equation must include the domain of dependence of the original differential equation.* For example, a right-moving wave (with  $a > 0$ ) has a solution whose time evolution at a particular point is governed by the spatial variation of the wave to the left of that point—not to the right. Therefore the numerical solution must make use of information to the left of the grid point, which Eqs. (2.16) and (2.18) do not. One can define more precisely which grid points should contribute to the solution by examining the characteristic curves of the differential equation, but for now it will be sufficient to state that one may include more points than are actually required, perhaps to improve accuracy, but the stability requirements will depend in detail on the particular scheme chosen. Note that the upwind scheme is so named because the points to be included in the first order approximation are "upwind" from the current grid point.

Assuming that  $a > 0$ , we find that Eq. (2.15) is stable provided  $0 \leq \sigma \leq 1$ , while Eq. (2.17) is stable for any  $\sigma \geq 0$ . If the largest stable  $|\sigma|$  is  $\sigma_{max}$ , we may use any  $\Delta t$  value satisfying

$$\Delta t \leq \sigma_{max} \frac{\Delta x}{|a|}. \quad (2.20)$$

Thus approximation (2.15) is stable for  $\Delta t \leq \Delta x/|a|$ , while (2.17) is stable for any  $\Delta t$ . Similar stability criteria apply to approximations (2.16) and (2.17) when  $a < 0$ .

### 2.2.2 Explicit vs. Implicit Methods

The approximation of Eq. (2.15) is an example of a *time explicit*, or simply *explicit*, method. An explicit method is one in which an unknown value at time step  $n+1$  appears at only one grid point in the formula (e.g.,  $U_i^{n+1}$ ), and is given explicitly in terms of the previous values at step  $n$ . The approximation of Eq. (2.17) is an example of a *time implicit*, or simply *implicit*, method. An implicit method is one in which the unknown values of  $U$  at step  $n+1$  appear at more than one grid point in the approximation, and are determined implicitly by a set of simultaneous equations, rather than by a set of independent explicit equations.

Explicit and implicit methods each have their advantages. Explicit methods are much simpler to implement, as they do not entail the solution of simultaneous equations. Explicit methods usually require much less time to evaluate, per time step, than implicit methods, because the simultaneous equations inherent in the implicit schemes usually

require lengthy calculations to solve. On the other hand, implicit methods are stable for much larger time steps (often infinite, as above) than explicit methods. However, the error in the time dependent numerical solution increases as some power of the time step, so that in general an implicit scheme would require roughly the same time step as a similar explicit scheme to achieve the same level of accuracy, but at a much higher cost in computer time. Thus explicit methods are almost always preferable for time dependent problems.

Nevertheless, there are situations in which implicit methods are preferable. One case is the solution of "stiff" problems, which contain large characteristic velocities whose corresponding effects are of minor importance. The time step for an explicit scheme is limited by the largest characteristic velocity, whether or not the associated phenomena play a major role in the solution. An implicit scheme may then be used with a time step small enough to follow the phenomena of interest (such as convection), but much larger than that dictated by the time scales of unimportant phenomena (such as sound waves). Flows at very small Mach numbers fit into this category.

Another case in which implicit methods are useful is in steady state flow models. One way to model a steady state flow problem is to pick a set of initial conditions and let the problem evolve to an equilibrium state. The time dependent solution is of no interest, and need not be accurate provided that the steady state solution obtained is correct. Once again, a small number of computationally expensive steps may be more efficient than a large number of inexpensive steps.

Implicit methods generally have to be tailored quite carefully to the problem at hand, while explicit methods can be made very general. Thus from now on the discussion will focus on explicit methods.

### 2.2.3 Two Popular Second Order Schemes

The first order upwind schemes suffer from two deficiencies. The first is low resolution. An initially sharp profile (such as a step function) is smeared out or "diffused" over many grid intervals as the solution progresses. This smearing tendency is known as numerical viscosity, and is a nonphysical effect (nonphysical because the original differential equation was inviscid).

The second deficiency concerns the nature of the upwind stability criteria. In subsonic fluid flow there is no simple upwind direction, as the flow has characteristic velocities in all directions. A direct application of the upwind scheme will therefore be unstable, unless the equations are put in characteristic form first, and each characteristic equation approximated by the appropriate upwind form. The characteristic form is useful for specifying boundary conditions, but is needlessly complex for other problems.

Finite difference schemes which make use of symmetrically located data points possess stability criteria which are independent of the flow direction. One early attempt at a symmetric method, which is still widely used, is the Lax-Wendroff scheme [5]. We start with a Taylor's series approximation for  $U_i^{n+1}$  about time  $t^n$ , truncated after the second order term:

$$U_i^{n+1} = U_i^n + \Delta t \left. \frac{\partial U}{\partial t} \right|_i^n + \frac{\Delta t^2}{2} \left. \frac{\partial^2 U}{\partial t^2} \right|_i^n. \quad (2.21)$$

Equation (2.14) may be solved by substituting  $-\partial f/\partial x$  for  $\partial U/\partial t$  in (2.21), and using Eq. (2.5) for the wave velocity. The result is the approximation

$$U_i^{n+1} = U_i^n - \Delta t \left. \frac{\partial f}{\partial x} \right|_i^n + \frac{\Delta t^2}{2} \frac{\partial}{\partial x} \left( a \frac{\partial f}{\partial x} \right) \Big|_i^n, \quad (2.22)$$

where  $a = a(U)$  in general. Making the spatially centered, second order finite difference approximations

$$\left. \frac{\partial f}{\partial x} \right|_i = \frac{1}{2\Delta x} (f_{i+1} - f_{i-1}), \quad (2.23)$$

$$\left. \frac{\partial}{\partial x} \left( a \frac{\partial f}{\partial x} \right) \right|_i = \frac{1}{\Delta x^2} [a_{i+1/2} (f_{i+1} - f_i) - a_{i-1/2} (f_i - f_{i-1})], \quad (2.24)$$

gives an explicit solution to Eq. (2.14) which is second order accurate in time and space. When applied to the linear wave equation, the Lax-Wendroff method gives

$$U_i^{n+1} = U_i^n - \frac{1}{2} \sigma (U_{i+1}^n - U_{i-1}^n) + \frac{1}{2} \sigma^2 (U_{i+1}^n - 2U_i^n + U_{i-1}^n), \quad (2.25)$$

with  $\sigma$  given by Eq. (2.19), which has a stability criterion independent of the sign of  $a$ :

$$\left| a \frac{\Delta t}{\Delta x} \right| \leq 1. \quad (2.26)$$

The Lax-Wendroff method is easily applied to single one dimensional wave equations. However, its extension to systems in one dimension, with an unknown variable vector  $u$  and vector flux function  $f(u)$ , entails the calculation of the Jacobian matrix  $\partial f/\partial u$  where the innocent-looking  $a$  appears in Eq. (2.22), a tedious if not impossible task.

MacCormack [6] came up with an apparently simpler method for the nonlinear systems case. MacCormack's method reduces to Eq. (2.25) for the linear wave equation, but is not the same as the Lax-Wendroff method for more complicated problems. The MacCormack method solution to Eq. (2.14) may be written

$$\begin{aligned} \tilde{U}_i &= U_i^n - \frac{\Delta t}{\Delta x} (f_{i+1}^n - f_i^n), \\ U_i^{n+1} &= U_i^n - \frac{\Delta t}{2\Delta x} (\tilde{f}_i - \tilde{f}_{i-1}) - \frac{\Delta t}{2\Delta x} (f_{i+1}^n - f_i^n), \\ &= \frac{1}{2} (U_i^n + \tilde{U}_i) - \frac{\Delta t}{2\Delta x} (\tilde{f}_i - \tilde{f}_{i-1}). \end{aligned} \quad (2.27)$$

This is a two step explicit method which does not require the Jacobian of the flux function. However, it is not a symmetric method: Eq. (2.27) uses a right direction one sided approximation to  $\partial f^n/\partial x$  and a left direction one sided approximation to  $\partial \tilde{f}/\partial x$ . One could have chosen the left direction approximation for the derivative of  $f^n$  and the right direction for  $\tilde{f}$ . The choice of direction for the terms is arbitrary, so long as they are opposed, but the two possible choices will give slightly different results when applied to the same nonlinear problem. MacCormack advocated switching the direction of differencing at successive time steps in order to restore symmetry. Switching entails cycling through  $2^m$  possible schemes in succession in  $m$  dimensions, which can lead to complications as difficult as those of the Lax-Wendroff scheme.

## 2.3 The Method of Lines

The preceding methods, while simple to formulate for single one dimensional wave equations, become quite complex and tricky to implement for multidimensional nonlinear systems such as the fluid equations. The difficulties stem from the use of one-sided difference approximations in the case of the upwind schemes, and from the simultaneous approximations of space and time derivatives in the Lax-Wendroff and MacCormack methods. These difficulties can be avoided by the *method of lines* approach, which is readily applicable to any time dependent partial differential equation solution.

We are given a set of partial differential equations in space and time, along with the initial data at time  $t = 0$ . Approximating the spatial derivatives with finite difference expressions in turn tells us how the solution changes in time at each grid point, allowing us to integrate the time derivatives to obtain the solution at a new time step.

More formally, suppose we have a system of equations describing the components of a solution vector  $\mathbf{u}$ . (For example, we might have  $\mathbf{u} = (\rho, m, e)$ , where  $\rho$  is the fluid density,  $m$  is the momentum density, and  $e$  is the energy density.) If the time derivatives of the components  $u_j$  appear only in the first degree, then the system can always be written as

$$\frac{\partial \mathbf{u}}{\partial t} = P\mathbf{u}, \quad (2.28)$$

where  $P$  is an operator involving any combination of the coordinates  $x$  and  $t$ , as well as the unknown variables  $u_j$  and their spatial derivatives, but no time derivatives of  $u_j$ . In the case of Eq. (2.14),  $\mathbf{u}$  is a vector with only one component  $u$ , and  $Pu = -\partial f / \partial x$ .

Now approximate all spatial derivatives in  $Pu$  with the appropriate finite difference formulas, yielding the numerical approximation  $(PU)_i$  (e.g., a spatially centered approximation such as  $(PU)_i = -(f_{i+1} - f_{i-1}) / 2\Delta x$ ). Then we have a *semi-discrete* equation for  $dU_i/dt$ , the time derivative of  $\mathbf{U}$  at grid point  $i$ :

$$\frac{dU_i}{dt} = (PU)_i. \quad (2.29)$$

In principle, any ordinary differential equation solution technique may be used to solve the coupled set of ordinary differential equations in Eq. (2.29), as long as the stability properties of the algorithm chosen allow reasonable step sizes  $\Delta t$ . Many such methods are available.

The reduction of a system of partial differential equations to semi-discrete form, followed by the integration of the system by an ordinary differential equation solver, is known as the *method of lines*.

One effective integration method for Eq. (2.29) is the classical, four step, fourth order

Runge-Kutta method [4], written as:

$$\begin{aligned}
 U_i^{(1)} &= U_i^n + \frac{1}{2}\Delta t(PU^n)_i, \\
 U_i^{(2)} &= U_i^n + \frac{1}{2}\Delta t(PU^{(1)})_i, \\
 U_i^{(3)} &= U_i^n + \Delta t(PU^{(2)})_i, \\
 U_i^{n+1} &= U_i^n + \frac{1}{6}\Delta t(PU^n + 2PU^{(1)} + 2PU^{(2)} + PU^{(3)})_i.
 \end{aligned} \tag{2.30}$$

This method requires the storage of the old step  $U_i^n$ , the current intermediate step  $U_i^{(k)}$ , and the running total of the sum of operators appearing in the last step.

The time error in (2.30) is  $O(\Delta t^4)$ . Since the maximum  $\Delta t$  is proportional to  $\Delta x$  because of the stability criterion (given below), the time integration contributes an error of  $O(\Delta x^4)$ . Thus the spatial approximations should also be fourth order accurate, or else some of the effort involved in the time integration is being wasted. If the spatial approximations are at best second order accurate (common in fluid problems), we should use a second order time stepping scheme which requires less work to perform than (2.30). The following four step, second order method is suited for such problems [7]:

$$\begin{aligned}
 U_i^{(1)} &= U_i^n + \frac{1}{4}\Delta t(PU^n)_i, \\
 U_i^{(2)} &= U_i^n + \frac{1}{3}\Delta t(PU^{(1)})_i, \\
 U_i^{(3)} &= U_i^n + \frac{1}{2}\Delta t(PU^{(2)})_i, \\
 U_i^{n+1} &= U_i^n + \Delta t(PU^{(3)})_i.
 \end{aligned} \tag{2.31}$$

Not only does Eq. (2.31) require less storage than Eq. (2.30), but its simpler structure allows all four steps to be performed by one master loop, using a different coefficient for  $\Delta t$  in each iteration.

Both the fourth order Runge-Kutta method of (2.30) and the second order method of (2.31) have the stability criterion

$$|\sigma| = \left| a \frac{\Delta t}{\Delta x} \right| \leq \sigma_{max} \tag{2.32}$$

for the linear wave problem. If a second order centered approximation is made to  $\partial u / \partial x$ , then  $\sigma_{max} = 2\sqrt{2}$ ; if a fourth order centered approximation is made, then  $\sigma_{max} = 2.06$ . (Note: when  $Pu$  is a linear operator, such as  $a \partial u / \partial x$ , with  $a = \text{constant}$ —and only then—Eq. (2.31) also gives a fourth order accurate time integration.)

## 2.4 Dissipation and Discontinuous Solutions

Consider the initial value problem

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0, \quad a = \text{constant} > 0; \tag{2.33}$$

$$u(x, 0) = u_0(x) = \begin{cases} 1 & x \leq 0, \\ 0 & x > 0. \end{cases} \quad (2.34)$$

The solution is a step function of unit height, moving with velocity  $a$ . We would like to solve this problem using the finite difference methods discussed so far.

This innocuous-seeming problem is in reality one of the most difficult wave problems to solve numerically. The techniques previously described give uniformly poor results at, say, a Courant number of  $\sigma = 0.5$ . The results fall into one of two categories: 1) solutions which are monotonic but badly smeared, with the original discontinuity spread out over many grid intervals, and 2) solutions which contain spurious oscillations, especially near the discontinuity, but where the discontinuity is more sharply resolved than in category 1. The first order (upwind) methods yield the diffuse monotone solutions, while the higher order methods yield the oscillatory solutions.

These results are explained by the following theorem [8]: *Any linear finite difference scheme which is guaranteed to preserve monotonicity is no more than first order accurate.*

This theorem is a major disappointment, as we would like to create high order solution methods which preserve the monotonicity of discontinuous solutions. The diffuse solutions produced by first order methods are usually inadequate; however, highly oscillatory solutions for discontinuous problems are equally inadequate. The theorem states that no linear finite difference scheme will satisfy the conflicting requirements of monotonicity and resolution. Therefore we must turn to nonlinear schemes for improvement. While the properties of nonlinear schemes can seldom be analyzed analytically, much can be accomplished by the careful blending of experience and linear theory.

We begin by examining more closely the first and second order approximations in semi-discrete form:

$$\frac{dU_i}{dt} = -\frac{1}{\Delta t} \sigma (U_i - U_{i-1}) \quad (\text{First order}), \quad (2.35)$$

$$= -\frac{1}{\Delta t} \frac{\sigma}{2} (U_{i+1} - U_{i-1}) \quad (\text{Second order}). \quad (2.36)$$

The choice of time integration is irrelevant for the moment, but Eq. (2.31) will do in practice. Note that Eq. (2.35) may be written as Eq. (2.36) plus a correction term:

$$\frac{dU_i}{dt} = \frac{1}{\Delta t} \left[ -\frac{\sigma}{2} (U_{i+1} - U_{i-1}) + \frac{|\sigma|}{2} (U_{i+1} - 2U_i + U_{i-1}) \right] \quad (\text{First order}). \quad (2.37)$$

(The above equation is in fact a general upwind scheme, which automatically switches to the appropriate direction based on the sign of  $a$ .) The correction term may be thought of as the finite difference approximation to the dissipative term

$$\frac{\partial}{\partial x} \left( \frac{|\sigma|}{2} \frac{\Delta x^2}{\Delta t} \frac{\partial u}{\partial x} \right),$$

with a diffusion coefficient defined by the Courant number  $\sigma$  and the grid parameters  $\Delta x$  and  $\Delta t$ . The added dissipation damps (i.e., prevents) the spurious oscillations which

would otherwise be generated by the second order centered difference approximation to  $\partial u / \partial x$ . This particular choice of diffusion coefficient ( $\frac{|\sigma| \Delta x^2}{2 \Delta t}$ ) is exactly that required to damp the oscillations completely, while a smaller value would not do so. This coefficient also smears (diffuses) the solution badly, and reduces the overall accuracy of the approximation to first order. In the limit as  $\Delta x \rightarrow 0$  and  $\Delta t \rightarrow 0$ , with  $\sigma = a \Delta t / \Delta x$  fixed, the dissipative term vanishes (as it must, for the finite difference approximation to remain consistent with the original inviscid equation), but it vanishes as a first order term.

The quest for a good nonlinear scheme may therefore be considered as a quest for a good diffusion coefficient. We can write the equation to be solved as

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = \frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right), \quad (2.38)$$

with the understanding that  $\kappa$  is nonzero only because our grid intervals are nonzero. In the limit as  $\Delta x$  and  $\Delta t$  vanish,  $\kappa$  must also vanish. Therefore we explicitly define  $\kappa \propto \Delta t$ , in order that  $\kappa$  vanish in the appropriate limit. (Why do we not define  $\kappa \propto \Delta x$  instead? Because to do so leads to confusion and the violation of an isotropy condition in multidimensional problems, as we'll see later. In addition, while  $\Delta t$  always has units of time, the spatial grid parameter may have different units in different problems—angular units, for example, in problems with cylindrical geometry. Thus it would be difficult to come up with a general expression for  $\kappa$  which is proportional to the grid spacing.) We also require that the relative sizes of the convective ( $a \partial u / \partial x$ ) and dissipative terms be independent of the time step, as indeed they are in Eq. (2.37). These requirements are met for

$$\kappa = k \Delta t \frac{a^2}{|\sigma|}, \quad (2.39)$$

where  $k$  is a dimensionless, non-negative constant. Note that  $\kappa$  is never less than zero, and is independent of the sign of  $a$ . The case  $k = 1/2$  recovers the monotone first order result of (2.37). The case  $0 < k < 1/2$  reveals that while a linear scheme may not achieve the best of both worlds, it can achieve the worst: an oscillatory first order scheme!

Note that the above scheme works just as well on a nonlinear equation, such as Burger's equation, where  $a(u) = u$ . Then  $a$ ,  $\kappa$ , and  $\sigma = a(u) \Delta t / \Delta x$  are functions of position, although  $\Delta t$  is not. In this case  $a \partial u / \partial x$  should be written as  $\partial f / \partial x$ ,  $f = u^2/2$ , in order to ensure conservation and the correct shock jumps (as in Chapter 1).

Eq. (2.39) may be converted into a nonlinear scheme by defining

$$\kappa = k \Delta t \frac{a^2}{|\sigma|} \nu, \quad (2.40)$$

where  $\nu$  depends on the local numerical solution  $U$ . We can define  $\nu$  in such a way as to satisfy  $\nu \leq 1$  always, to have  $\nu \approx 1$  near discontinuities and oscillatory regions, and to vanish as a first order quantity in regions where  $U$  is a smooth, continuous function. In finite difference form we write

$$\frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) \Big|_i = \frac{1}{\Delta x^2} \left[ \kappa_{i+1/2} (U_{i+1} - U_i) - \kappa_{i-1/2} (U_i - U_{i-1}) \right], \quad (2.41)$$

for which

$$\kappa_{i+1/2} = \frac{1}{2}(\kappa_i + \kappa_{i+1}), \quad (2.42)$$

$$\kappa_i = k\Delta t \frac{a_i^2}{|\sigma_i|} \nu_i, \quad \sigma_i = a_i \frac{\Delta t}{\Delta x}. \quad (2.43)$$

Of the many possibilities we could pick for  $\nu_i$ , one of the most useful is

$$\nu_i = \frac{|U_{i+1} - 2U_i + U_{i-1}|}{|U_{i+1} - U_i| + |U_i - U_{i-1}|}. \quad (2.44)$$

This definition has  $\nu_i = 1$  if  $U_i$  is a local maximum or minimum. Thus  $\kappa_{i+1/2}$  will be a maximum only if  $U_i$  and  $U_{i+1}$  are both local extremes, which is by definition a spurious oscillation to be damped. Note that the *local* wave speed  $a_i$  and Courant number  $\sigma_i$  appear, so that the above prescription may be applied to the general case of spatially varying wave velocities. The quantity  $a_i^2/|\sigma_i| \propto |a_i|$ ; hence the diffusion coefficient is larger when the wave velocity is larger, which is as it should be, since the solution (and spurious oscillations) will evolve more quickly in regions where  $a_i$  is large.

The constant  $k$  sets an upper limit to the diffusion coefficient, and is left as a free parameter to be set by the user. Different problems will give the best results for different  $k$  values. The choice  $k = 1/2$  should eliminate spurious oscillations; however, in many cases  $k = 1/2$  will be excessive, and a smaller value should be chosen.

The preceding analysis has focused on the choice of a second order central difference approximation for the  $\partial u/\partial x$  (or  $\partial f/\partial x$ ) term. One could choose the fourth order approximation (2.11), in which case the above scheme would still reduce to a first order solution for  $\nu \equiv 1$ , but which is not guaranteed to be monotonic. Nevertheless, one finds in practice that those oscillations which do occur are more easily damped (i.e., require smaller  $k$  values) than is the case when second order approximations are made.

## 2.5 The Method of Lines in Two Dimensions

The extension of the preceding techniques to two or more dimensions is straightforward. We begin with a single conservation law in two spatial dimensions:

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} = 0, \quad f = f(u), \quad g = g(u), \quad (2.45)$$

or

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} + b \frac{\partial u}{\partial y} = 0, \quad a = \frac{df}{du}, \quad b = \frac{dg}{du}. \quad (2.46)$$

The two equations are equivalent. If  $a$  and  $b$  are constant, the solution is

$$u(x, y, t) = u_0 \left( \frac{ax + by}{a^2 + b^2} - t \right), \quad (2.47)$$

which is a wave moving at constant speed, with velocity components  $a$  in the  $x$  direction and  $b$  in the  $y$  direction.



The second order semi-discrete approximation to Eq. (2.45) is

$$\frac{dU_{ij}}{dt} = -\frac{f_{i+1j} - f_{i-1j}}{2\Delta x} - \frac{g_{ij+1} - g_{ij-1}}{2\Delta y}, \quad (2.48)$$

in the absence of dissipation. The grid points are assumed to be uniformly spaced, with  $x_i = i\Delta x$ ,  $y_j = j\Delta y$ , and  $U_{ij}^n \equiv U(x_i, y_j, t^n)$ .

Dissipation is introduced by adding diffusive terms to Eq. (2.45) in the form

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} = \frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial u}{\partial y} \right), \quad (2.49)$$

where  $\kappa \rightarrow 0$  as  $\Delta t \rightarrow 0$ , as before. We define  $\kappa$  in terms of the local Courant number  $\sigma_{ij}$ ,

$$\sigma_{ij} = \Delta t \left( \frac{|a_{ij}|}{\Delta x} + \frac{|b_{ij}|}{\Delta y} \right), \quad (2.50)$$

and the largest local velocity component  $c_{ij} = \max(|a_{ij}|, |b_{ij}|)$ :

$$\kappa_{ij} = k \Delta t \frac{c_{ij}^2}{\sigma_{ij}} \nu_{ij}, \quad (2.51)$$

where a useful (but not unique) definition for  $\nu_{ij}$  is

$$\nu_{ij} = \max \left( \frac{|U_{i+1j} - 2U_{ij} + U_{i-1j}|}{|U_{i+1j} - U_{ij}| + |U_{ij} - U_{i-1j}|}, \frac{|U_{ij+1} - 2U_{ij} + U_{ij-1}|}{|U_{ij+1} - U_{ij}| + |U_{ij} - U_{ij-1}|} \right). \quad (2.52)$$

The same definition for  $\kappa$  is used in both dissipative terms in Eq. (2.49). This uniqueness in the definition of  $\kappa$  is required by the transformation properties of scalar fields, a subject which will be taken up in detail in Chapter 4.

The second order semi-discrete approximation to Eq. (2.49) is then

$$\begin{aligned} \frac{dU_{ij}}{dt} = & -\frac{f_{i+1j} - f_{i-1j}}{2\Delta x} - \frac{g_{ij+1} - g_{ij-1}}{2\Delta y} \\ & + \frac{1}{\Delta x^2} [\kappa_{i+1/2j}(U_{i+1j} - U_{ij}) - \kappa_{i-1/2j}(U_{ij} - U_{i-1j})] \\ & + \frac{1}{\Delta y^2} [\kappa_{ij+1/2}(U_{ij+1} - U_{ij}) - \kappa_{ij-1/2}(U_{ij} - U_{ij-1})], \end{aligned} \quad (2.53)$$

where

$$\kappa_{i+1/2j} = \frac{1}{2}(\kappa_{ij} + \kappa_{i+1j}), \quad \kappa_{ij+1/2} = \frac{1}{2}(\kappa_{ij} + \kappa_{ij+1}). \quad (2.54)$$

The stability properties of this scheme are the same as for the one dimensional case of section 2.3, and with  $\max \sigma_{ij} \leq \sigma_{max}$ , for  $\sigma$  as defined by Eq. (2.50), and  $\sigma_{max}$  as given in section 2.3.

## 2.6 Exercises

1. Using the fourth order approximation to  $df/dx|_i$  given in Eq. (2.9), compute the sixth order approximation.
2. Compute second and third order one sided approximations to  $df/dx|_i$ , starting with the first order one sided approximation of Eq. (2.6).

The following exercises are numerical solutions of the two initial value problems

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0, \quad f = au, \quad a = 1,$$

$$u(x, 0) = u_1(x) \quad \text{or} \quad u_2(x),$$

$$u_1(x) = e^{-[(x-0.25)/0.1]^2},$$

$$u_2(x) = \begin{cases} 1 & x \leq 0.25, \\ 0 & x > 0.25. \end{cases}$$

In all cases let  $\Delta x = 0.01$ ,  $x_i = i\Delta x$ , and compute the numerical solution  $U_i$  for grid points  $i = 0$  through 100. Define initial values for  $U_i$  for  $i = -2$  through 102 from the initial conditions, but do not recompute  $U_{-2}$ ,  $U_{-1}$ ,  $U_{101}$ , or  $U_{102}$  at the new time steps. (In other words, hold the boundary values fixed with time.) Compute 100 time steps at a Courant number  $\sigma = 1/2$ . At time step 100, plot the analytic solution  $u_1(x - at)$  or  $u_2(x - at)$  as a continuous unmarked curve, and the numerical solution  $U_i^n$ ,  $n = 100$ , as dots at the positions  $(x_i, U_i^n)$ ,  $i = 0, \dots, 100$ . Use the computer to plot as well as compute the results.

3. One sided (upwind) scheme (2.15) with  $u_1$  and  $u_2$  as initial data.
4. Lax-Wendroff method (2.22) with  $u_1$  and  $u_2$  as initial data.
5. Method of lines: scheme (2.31) with  $(PU)_i = -(f_{i+1} - f_{i-1})/2\Delta x$ , using  $u_1$  and  $u_2$  as initial data.
6. Same as 3, but adding the dissipative term of (2.41) to the right hand side (i.e., to  $(PU)_i$  as defined in problem 3), with  $\kappa$  given by Eqs. (2.42)–(2.44), and  $k = 0, 0.2$ , and 0.5.
7. Same as 6, but using the fourth order approximation (2.11) to  $\partial f/\partial x$ .
8. Same as 3, but using Burger's equation in conservative form (1.22) and the initial value problem of Exercise 3, Chapter 1. Compute the time step size at the beginning of each time step according to  $\Delta t = \sigma\Delta x/U_{max}$ , where  $U_{max}$  is the largest absolute value of the numerical solution ( $\max_{i=0}^{100} |U_i^n|$ ) on the grid at the beginning of the current time step. The left boundary condition must now be changed to one of antisymmetry, given by  $U_{-1} = -U_1$ ,  $U_{-2} = -U_2$ . Does the numerical solution match the analytical solution?

# Chapter 3

## Stability Analysis

Chapter 2 presented several approximate finite difference solutions for one dimensional conservation laws. The criteria used to select an appropriate technique are stability, accuracy, and efficiency. Of these stability is the most important, as the formal accuracy and efficiency of a method are irrelevant if the method is unstable in practice. The stability limits for the methods in Chapter 2 were stated without proof. In this chapter I will present a general technique for determining the stability of finite difference approximations for wave equations.

### 3.1 The Consistency Condition and the Lax Equivalence Theorem

The partial differential equations we wish to solve may be written in the general form

$$\frac{\partial \mathbf{u}}{\partial t} = P\mathbf{u}, \quad (3.1)$$

where  $P$  is an operator which acts on  $\mathbf{u}$  to give its time derivative. The quantity  $P\mathbf{u}$  may be nonlinear and contain any combination of powers of the spatial coordinates, time, or unknown elements  $u_k$ , or any spatial derivatives of these combinations, but may not contain time derivatives of  $\mathbf{u}$ .

As in Chapter 2, we consider only the pure initial value problem, for which the initial data are given, and the time dependent solution is to be obtained, over an infinite spatial domain with no boundaries or boundary conditions.

Replacing the spatial derivatives in  $P$  with suitable finite difference approximations yields the semi-discrete approximation

$$\frac{dU_i}{dt} = (PU)_i, \quad (3.2)$$

where  $U_i$  is the approximate solution for  $U$  at the  $i$ th grid point.

Given data at time level  $t^n$ , we integrate Eq. (3.2) to time level  $t^{n+1} = t^n + \Delta t$ . Thus the new value of  $U_i^{n+1}$  is some function of the old values  $U_{i+k}^n$ ,  $k = -\infty, \dots, \infty$ . The

functional relationship between the new and old values may be written

$$U_i^{n+1} = C(\Delta t)U_i^n, \quad (3.3)$$

where the operator  $C(\Delta t)$  acts on  $U_i$  and depends on  $\Delta t$ .

We know from section (2.1) that the quantity  $(U_i^{n+1} - U_i^n) / \Delta t$  is an approximation to the time derivative of  $U_i$ , hence

$$\frac{C(\Delta t)U^n - U^n}{\Delta t}$$

must be an approximation to  $PU$ .

The *consistency condition* therefore requires that

$$\left\| \left\{ \frac{C(\Delta t) - I}{\Delta t} - P \right\} U_i(t) \right\| \rightarrow 0 \text{ as } \Delta t \rightarrow 0, \quad (3.4)$$

where  $\|f\|$  is any valid norm of  $f$  and  $I$  is the identity operator [5].

The consistency condition looks imposing, but it is simply a formal statement of an intuitively meaningful concept, namely that the finite difference approximations which are used in the numerical solution of a differential equation must yield that equation in the limit as all grid spacings go to zero (i.e., as  $\Delta x \rightarrow 0$  and  $\Delta t \rightarrow 0$  for the methods of Chapter 2).

The consistency condition is automatically satisfied by any one-to-one replacement of derivatives by valid finite difference approximations, so the insistence on consistency may seem redundant. However, we saw in Chapter 2 that dissipative terms were required in the finite difference solution to discontinuous problems, even though these terms do not represent finite difference approximations to derivative terms appearing in the original differential equations. Thus an approximation containing these added dissipative terms must be defined in such a way that the dissipation vanishes in the limit of zero grid spacing in order to retain consistency (otherwise our finite difference method is solving a problem different from the one whose solution we want). The dissipative terms in section 2.4 vanish as  $\Delta t \rightarrow 0$ , because  $\kappa \propto \Delta t$ . If we had defined  $\kappa$  so that  $\kappa \neq 0$  as  $\Delta t \rightarrow 0$ ,  $\Delta x \rightarrow 0$ , then the approximation would have been inconsistent, and guaranteed *not* to converge to the correct answer in this limit.

The definition of consistency given above leads to the *Lax Equivalence Theorem* [5]:

*Given a properly posed initial-value problem and a finite difference approximation to it that satisfies the consistency condition, stability is the necessary and sufficient condition for convergence.*

The proof of the theorem assumes  $P$  to be a linear operator, but in practice the same result is observed to hold for nonlinear systems as well, provided the dissipation is chosen properly.

Having established that stable and consistent schemes will converge to the correct answer, we proceed next to define and analyze the stability of finite difference approximations.

## 3.2 The Von Neumann Method for Stability Analysis

According to Eq. (3.3), the operator  $C(\Delta t)$  advances the solution from time  $t$  to time  $t + \Delta t$ . Thus initial data  $U_i^0$  yield data at time  $t^n = n\Delta t$  through the repeated application of  $C(\Delta t)$ ,

$$U_i^n = [C(\Delta t)]^n U_i^0. \quad (3.5)$$

A scheme is stable if there exists a  $\tau > 0$  such that the set of operators  $[C(\Delta t)]^n$  is bounded for  $0 \leq \Delta t \leq \tau$ . In other words, the numerical solution may not grow without bound (provided that the correct solution does not). Conversely, a numerical scheme which is unstable will exhibit unbounded growth, and this growth is virtually always exponential.

Note that computing a bound for  $[C(\Delta t)]^n$  is not trivial, as  $C(\Delta t)$  is an operator, not a number. Fortunately, a straightforward technique for transforming the operator  $C(\Delta t)$  into a number does exist, when  $C(\Delta t)$  is a linear operator. The technique is known as the Von Neumann method and is described below.

### 3.2.1 Fourier Analysis and the Linear Wave Equation

We consider once again the linear wave equation

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0, \quad a = \text{constant}, \quad (3.6)$$

and examine the behavior of the numerical solution for  $u$ . Fourier analysis turns out to be a convenient tool for this examination. The Fourier transform of a function  $f(x)$  is the frequency spectrum of the function,  $\hat{f}(\omega)$ , and is a function of the frequency  $\omega$ . If  $f = f(x, t)$  and we take the Fourier transform of the  $x$  dependence, the spectrum is  $\hat{f}(\omega, t)$ . If in turn  $\hat{f}(\omega, t)$  is a monotonically increasing function of  $t$  for some frequency  $\omega_0$ ,  $f(x, t)$  will be an unbounded function, since the frequency component  $\omega_0$  grows without bound.

The Fourier transform of the  $x$  dependence of a function  $u(x, t)$  may be written

$$\mathcal{F}\{u(x, t)\} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega x} u(x, t) dx \equiv \hat{u}(\omega, t), \quad (3.7)$$

and is finite if  $u(x, t) \rightarrow 0$  sufficiently quickly as  $x \rightarrow \pm\infty$ , which we will assume throughout.

The derivative  $\partial u / \partial x$  transforms according to

$$\mathcal{F}\left\{\frac{\partial}{\partial x} u(x, t)\right\} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega x} \frac{\partial}{\partial x} u(x, t) dx \equiv i\omega \hat{u}(\omega, t), \quad (3.8)$$

which is obtained upon integration by parts.

Taking the Fourier transform of the linear wave equation (3.6) gives

$$\frac{\partial \hat{u}}{\partial t} + i\omega a \hat{u} = 0. \quad (3.9)$$

Notice that Eq. (3.9) is an ordinary differential equation for any particular choice of  $\omega$ . The effect of the Fourier transform has been to replace a single partial differential equation with an infinite number of ordinary differential equations.

The solution of Eq. (3.9) is

$$\hat{u}(\omega, t) = e^{-i\omega a t} \hat{u}(\omega, 0), \quad (3.10)$$

and therefore

$$\left| \frac{\hat{u}(\omega, t)}{\hat{u}(\omega, 0)} \right| = 1. \quad (3.11)$$

Although the phases of the components of the frequency spectrum change with time, their magnitudes do not. Indeed, this is the behavior we would expect, since we know the solution to be a traveling wave of constant shape.

### 3.2.2 Fourier Analysis for Finite Difference Approximations

Previously we have taken  $U_i^n$  to be the numerical approximation to the exact solution at the point  $(x_i, t^n)$ . For the remainder of this chapter, we will adopt a slightly different, but equivalent, interpretation, and assume that  $U_i^k$  is a function defined by

$$U_{i+k}^n \equiv U(x + k\Delta x, t) \Big|_{x_i}^{t^n}, \quad (3.12)$$

which we happen to sample at discrete points. Thus any derivative approximation, such as

$$\frac{\partial U}{\partial x} \Big|_i^n \approx \frac{U_{i+1}^n - U_{i-1}^n}{2\Delta x} \equiv \frac{U(x + \Delta x, t^n) - U(x - \Delta x, t^n)}{2\Delta x} \Big|_{x_i}, \quad (3.13)$$

is also a continuous function, and we may compute its Fourier transform.

Assuming  $\Delta x$  to be a fixed constant, we have

$$\mathcal{F}\{U(x, t)\} = \hat{U}, \quad (3.14)$$

$$\mathcal{F}U(x + k\Delta x, t) = e^{ik\xi} \hat{U}, \quad \xi \equiv \omega \Delta x. \quad (3.15)$$

The variable  $\xi$  is referred to as the dimensionless frequency, and is an angular quantity (hence dimensionless).

We can now compute the Fourier transforms of finite difference approximations. Let  $\frac{1}{\Delta x} \delta_x^{(m)} U_i$  be an  $m$ th order approximation to  $\partial U / \partial x|_i$ . Then we represent the one sided approximations by

$$\delta_x^{(1)-} U_i = U_i - U_{i-1}, \quad \delta_x^{(1)+} U_i = U_{i+1} - U_i, \quad (3.16)$$

and the centered approximations by

$$\delta_x^{(2)} U_i = \frac{1}{2}(U_{i+1} - U_{i-1}), \quad (3.17)$$

$$\delta_x^{(4)} U_i = \frac{1}{12}[8(U_{i+1} - U_{i-1}) - (U_{i+2} - U_{i-2})]. \quad (3.18)$$

The second derivative,  $\partial^2 U / \partial x^2|_i$  is approximated by  $\frac{1}{\Delta x^2} \delta_x^{(2)} U_i$ , to order  $m$ , and we have

$$\delta_x^{(2)} U_i = U_{i+1} - 2U_i + U_{i-1}. \quad (3.19)$$

The transforms are

$$\mathcal{F}\{\delta_x^{(1)-} U_i\} = (1 - e^{-i\xi}) \hat{U}, \quad \mathcal{F}\{\delta_x^{(1)+} U_i\} = (e^{i\xi} - 1) \hat{U}, \quad (3.20)$$

$$\mathcal{F}\{\delta_x^{(2)} U_i\} = (i \sin \xi) \hat{U}, \quad (3.21)$$

$$\mathcal{F}\{\delta_x^{(4)} U_i\} = i \frac{1}{6} [8 \sin \xi - \sin(2\xi)] \hat{U}, \quad (3.22)$$

$$\mathcal{F}\{\delta_x^{(2)} U_i\} = -4 \sin^2(\xi/2) \hat{U}. \quad (3.23)$$

### 3.2.3 Stability Condition for Numerical Methods

We can now state the Von Neumann stability condition for numerical approximations to the linear wave equation. All one step linear finite difference solutions to the linear wave equation (3.6), implicit or explicit, can be written as

$$\sum_{k=-\infty}^{\infty} l_k U_{i+k}^{n+1} = \sum_{k=-\infty}^{\infty} r_k U_{i+k}^n, \quad (3.24)$$

where the  $l_k$  and  $r_k$  are constants. Taking the Fourier transform of Eq. (3.24) gives

$$\left( \sum_{k=-\infty}^{\infty} l_k e^{ik\xi} \right) \hat{U}^{n+1} = \left( \sum_{k=-\infty}^{\infty} r_k e^{ik\xi} \right) \hat{U}^n, \quad (3.25)$$

from which we see

$$\hat{U}^{n+1} = g(\xi) \hat{U}^n, \quad (3.26)$$

$$g(\xi) \equiv \frac{\sum_{k=-\infty}^{\infty} r_k e^{ik\xi}}{\sum_{k=-\infty}^{\infty} l_k e^{ik\xi}}, \quad (3.27)$$

where  $g(\xi)$  is known as the *Fourier amplification factor*.

The Von Neumann stability condition is the following [5]: *Stability of finite difference approximation (3.24) requires that  $g(\xi)$ , as defined by Eq. (3.27), satisfy*

$$|g(\xi)| \leq 1, \quad \text{for all } \xi \text{ in } -\pi \leq \xi \leq \pi. \quad (3.28)$$

Otherwise the numerical solution grows exponentially with the number of time steps.<sup>1</sup>

The preceding formalism may appear complicated, but is simple to implement in practice, as the following examples show.

<sup>1</sup>A more general condition allows for exponential growth when such growth is a valid solution, and requires  $g(\xi) \leq 1 + O(\Delta t)$  [5]. This situation occurs when a source term  $bu$  is added to the right hand side of (3.6). For most problems condition (3.28) is sufficiently general, and will be used in these notes.

### 3.3 Simple Upwind Schemes

Let us first consider the upwind schemes of section 2.2.1. The Fourier transform of Eq. (2.15) is

$$\hat{U}^{n+1} = [1 - \sigma(1 - e^{-i\xi})]\hat{U}^n, \quad (3.29)$$

$$g(\xi) = 1 - \sigma(1 - e^{-i\xi}), \quad (3.30)$$

$$= 1 - \sigma(1 - \cos \xi) - i\sigma \sin \xi. \quad (3.31)$$

Multiplying Eq. (3.31) by its complex conjugate gives the square of the absolute magnitude of  $g$  as

$$|g(\xi)|^2 = 1 - 4\sigma(1 - \sigma) \sin^2(\xi/2). \quad (3.32)$$

The worst case has  $\xi = \pi$ , for which

$$|g(\pi)|^2 = 1 - 4\sigma(1 - \sigma) \leq 1, \quad (3.33)$$

$$\sigma(1 - \sigma) \geq 0, \quad (3.34)$$

and we must have  $0 \leq \sigma \leq 1$  for approximation (2.15) to be stable. A similar calculation shows that the stability bounds for approximation (2.16) is  $-1 \leq \sigma \leq 0$ . Thus the stability of the explicit upwind schemes depends on the sign of the velocity  $a$ .

Consider next the implicit upwind scheme of Eq. (2.17). Its Fourier transform is

$$\hat{U}^{n+1} = \hat{U}^n - \sigma(1 - e^{-i\xi})\hat{U}^{n+1}, \quad (3.35)$$

$$g = 1 - \sigma(1 - e^{-i\xi})g, \quad (3.36)$$

$$g(\xi) = \frac{1}{1 + \sigma(1 - \cos \xi) + i\sigma \sin \xi}, \quad (3.37)$$

$$|g(\xi)|^2 = \frac{1}{1 + 4\sigma(1 + \sigma) \sin^2(\xi/2)}. \quad (3.38)$$

Again the worst case occurs at  $\xi = \pi$ , and the condition  $|g(\xi)| \leq 1$  implies

$$\sigma(1 + \sigma) \geq 0, \quad (3.39)$$

and the method is stable for any  $\sigma \geq 0$ . Similarly, approximation (2.18) is stable for any  $\sigma \leq 0$ .

### 3.4 Simple Centered Methods

The simplest centered method we can have is the approximation

$$U_i^{n+1} = U_i^n - \frac{1}{2}\sigma(U_{i+1}^n - U_{i-1}^n). \quad (3.40)$$



The Fourier transform of (3.40) gives

$$g(\xi) = 1 - i\sigma \sin \xi, \quad (3.41)$$

$$|g(\xi)|^2 = 1 + \sigma^2 \sin^2 \xi, \quad (3.42)$$

so that approximation (3.40) is unconditionally unstable!

In Chapter 2 we found a dissipative term which, when added to the simple centered difference approximation, produced an upwind scheme which we now know to be stable for suitable time steps. The dissipative term is given in Eq. (2.37), and a first order time integration of (2.37) is

$$U_i^{n+1} = U_i^n - \frac{1}{2}\sigma(U_{i+1}^n - U_{i-1}^n) + \frac{1}{2}|\sigma|(U_{i+1}^n - 2U_i^n + U_{i-1}^n). \quad (3.43)$$

The Fourier transform of (3.43) gives

$$g(\xi) = 1 - |\sigma|(1 - \cos \xi) - i\sigma \sin \xi, \quad (3.44)$$

$$|g(\xi)|^2 = 1 + 4(\sigma^2 - |\sigma|) \sin^2(\xi/2), \quad (3.45)$$

and the stability condition is

$$\sigma^2 - |\sigma| \leq 0, \quad (3.46)$$

which is satisfied for  $|\sigma| \leq 1$ , and is independent of the sign of the velocity, unlike the original one-sided schemes.

We conclude that adding dissipation to a centered scheme which is originally unstable may produce a stable scheme. Thus we now consider a more general scheme of the form

$$U_i^{n+1} = U_i^n - \frac{1}{2}\sigma(U_{i+1}^n - U_{i-1}^n) + \frac{1}{2}\alpha(U_{i+1}^n - 2U_i^n + U_{i-1}^n), \quad (3.47)$$

where  $\alpha = \kappa \Delta t / \Delta x^2$  and  $\kappa$  is a constant diffusion coefficient, as in Eq. (2.38). The Fourier transform of Eq. (3.47) gives

$$g = 1 - i\sigma \sin \xi - 2\alpha(1 - \cos \xi), \quad (3.48)$$

$$|g(\xi)|^2 = 1 - 8\alpha \sin^2(\xi/2) + 16\alpha^2 \sin^4(\xi/2) + \sigma^2 \sin^2 \xi. \quad (3.49)$$

The condition  $|g(\xi)| \leq 1$  yields the equation

$$f(\xi) \equiv [2\alpha - \sigma^2 + (\sigma^2 - 4\alpha^2) \sin^2(\xi/2)] \sin^2(\xi/2) \geq 0 \text{ for all } \xi. \quad (3.50)$$

Eq. (3.50) specifies a relationship between  $\alpha$  and  $\sigma$ . Analyzing (3.50) in detail serves no purpose for the present, but for a given  $\sigma$  it puts lower and upper limits on the range of  $\alpha$  values which will lead to a stable approximation, and it defines a maximum value of  $|\sigma|$  above which any approximation will be unstable for any value of  $\alpha$ .

### 3.5 The Lax-Wendroff and MacCormack Methods

The Lax-Wendroff and MacCormack methods yield Eq. (2.25) when applied to the linear wave equation. The corresponding Fourier transform gives

$$g(\xi) = 1 - i\sigma \sin \xi + \sigma^2(1 - \cos \xi). \quad (3.51)$$

Using Eq. (3.50) with  $\alpha = \sigma^2/2$  gives

$$(\sigma^2 - \sigma^4) \sin^2(\xi/2) \geq 0, \quad (3.52)$$

or  $|\sigma| \leq 1$  for stability. These methods have the same stability limit as Eq. (3.43), although Eq. (3.43) is a first order accurate method, while the Lax-Wendroff and MacCormack schemes are second order accurate.

### 3.6 The Method of Lines

In the previous sections we have analyzed the stability of a method by writing the new value of  $U$ ,  $U_i^{n+1}$ , explicitly in terms of the old values  $U_i^n$ . Obtaining such an expression for a method of lines integration such as (2.30) or (2.31) is a tedious business, due to the many substitutions (substeps) involved. It is simpler to take the Fourier transform of the semi-discrete form first, and then impose a time integration algorithm [9].

We'll begin by considering the semi-discrete form of the linear wave equation, with added dissipation given by formulas (2.39) and (2.41),

$$\frac{dU_i}{dt} = -\frac{a}{\Delta x} \delta_x^{(m)} U_i + \frac{\kappa}{\Delta x^2} (U_{i+1} - 2U_i + U_{i-1}), \quad (3.53)$$

$$\kappa = k\Delta t \frac{a^2}{|\sigma|}, \quad (3.54)$$

where  $\delta_x^{(m)}$  is an  $m$ th order undivided difference operator, as given in equations (3.16)–(3.18). Eq. (3.53) may be written

$$\frac{dU_i}{dt} = \frac{1}{\Delta t} [-\sigma \delta_x^{(m)} U_i + k|\sigma| (U_{i+1} - 2U_i + U_{i-1})], \quad (3.55)$$

and its Fourier transform is

$$\frac{d\hat{U}}{dt} = \frac{1}{\Delta t} \Lambda \hat{U}, \quad (3.56)$$

$$\Lambda = -i\sigma P^{(m)}(\xi) - 4k|\sigma| \sin^2(\xi/2), \quad (3.57)$$

while the functions  $P^{(m)}(\xi)$  are

$$P^{(2)}(\xi) = \sin(\xi), \quad P^{(4)}(\xi) = \frac{1}{6} [8 \sin(\xi) - \sin(2\xi)]. \quad (3.58)$$

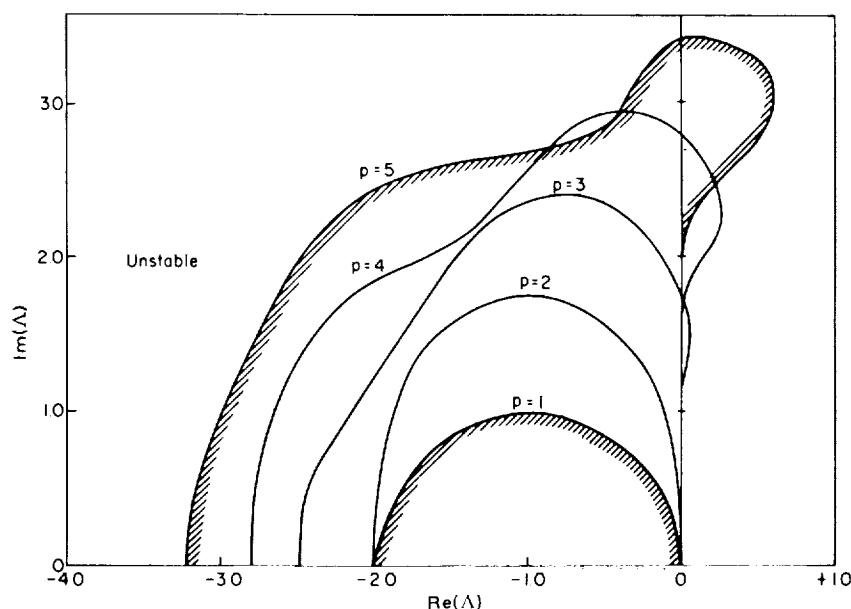


Figure 3.1: Stability regions for Runge-Kutta methods of order  $p$ . Copyright © 1971 by Academic Press, Inc. Reprinted by permission of Academic Press, Inc.

At this point we have two options. The first is to perform the time integration of (3.56) with either method (2.30) or (2.31), both of which give

$$g = 1 + \Lambda + \frac{1}{2}\Lambda^2 + \frac{1}{6}\Lambda^3 + \frac{1}{24}\Lambda^4. \quad (3.59)$$

The condition  $|g(\xi)| \leq 1$  defines a region in the complex plane known as the *stability region*, such that the method is stable if  $\Lambda$  lies within the stability region.

Much of the effort of obtaining a stability limit has so far been avoided by performing the Fourier transform before the time integration. However, determining the stability limit for  $\Lambda$  remains a non-trivial task, and a desire to avoid the effort involved leads us to the second option, which is to look up the stability limit of our time integration for Eq. (3.56) in a book on the numerical solution of ordinary differential equations.

Page 120 of the book by Lapidus and Seinfeld [10], reproduced here as Figure 3.1, gives stability regions for several methods. The figure shows the stability regions in the complex plane of  $\Lambda$  for Runge-Kutta methods of order  $p$ ,  $p = 1, \dots, 5$ . The  $p = 4$  curve applies for methods (2.30) and (2.31). This curve has imaginary intercepts at  $z = \pm 2\sqrt{2}i$ , and real intercepts at  $z = 0, -2.785$ . The symmetry of the curve about the real axis implies that the sign of the velocity  $a$  has no effect on the stability limits.

If  $k = 0$ , no dissipation is added and  $\Lambda = -i\sigma P^{(m)}(\xi)$  is purely imaginary, and must lie in  $-i2\sqrt{2} \leq \Lambda \leq i2\sqrt{2}$ . Hence

$$|\sigma P^{(m)}(\xi)| \leq 2\sqrt{2}, \quad (3.60)$$

and the maximum allowed value of  $\sigma$  is determined by the largest value of  $P^{(m)}(\xi)$ . We quickly determine that  $P_{max}^{(2)} = 1$ , and  $P_{max}^{(4)} = 1.3722$ , hence  $\sigma \leq 2\sqrt{2}$  for stability if a second order approximation to  $\partial u / \partial x$  is made, and  $\sigma \leq 2.0612$  if a fourth order approximation is made. (In both cases  $k = 0$ . Dissipation will decrease the stability limit even though it improves the quality of the solution.)

At the other extreme we consider the purely dissipative problem, with  $a = \sigma = 0$ , and replace  $k|\sigma|$  in (3.57) by  $\kappa\Delta t / \Delta x^2$ . Then  $\Lambda = -4\kappa\frac{\Delta t}{\Delta x^2} \sin^2(\xi/2)$ , and  $-2.785 \leq \Lambda \leq 0$ , from which we see that  $\kappa\Delta t / \Delta x^2 \leq 0.6963$  for stability. In real diffusion or heat conduction problems, where  $\kappa$  is some nonzero function of the solution  $u$ , the maximum stable time step is proportional to the square of the grid spacing. Reducing the grid spacing by a factor of two decreases the allowed time step by a factor of four. A finely spaced mesh may therefore require a prohibitively small time step for an explicit scheme to be stable, which suggests that an implicit scheme might be more efficient, though considerably more difficult to implement.

For the added dissipation we are considering here,  $\kappa\Delta t / \Delta x^2 = k|\sigma|$ , which vanishes as  $\sigma \rightarrow 0$ , so we cannot obtain a purely dissipative problem while  $\sigma$  is nonzero. However, if  $\sigma$  is sufficiently small, we can make  $k$  large enough that the second term of Eq. (3.57) dominates over the first, and we may conclude that  $k$  is restricted by the requirement  $k|\sigma| \leq 0.6963$  for stability.

A general expression relating the maximum value of  $k$  as a function of the Courant number  $\sigma$  probably cannot be derived analytically, but is not really necessary. If  $|\sigma|$  does not exceed roughly half of its upper limit, one can in practice make  $k$  large enough to damp any oscillations. The practical condition is to compute the time step from

$$\Delta t = \Delta x \frac{|\sigma|}{|a|}, \quad (3.61)$$

where  $\sigma$  is a Courant number which is less than the maximum value, and to set  $k$  to an optimum value obtained by experimentation (e.g.,  $|\sigma| = 1$ ,  $k = 0.3$ ).

### 3.7 Stability Analysis in Two Dimensions

Stability analysis for two or more dimensions is very similar to the one dimensional case, and we can use the one dimensional results with only slight modifications. We start with the Fourier transform in two dimensions  $(x, y)$  of a function  $u(x, y, t)$ , which may be defined

$$\mathcal{F}\{u(x, y, t)\} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy e^{-i(\omega_x x + \omega_y y)} u(x, y, t) \equiv \hat{u}(\omega_x, \omega_y, t). \quad (3.62)$$

It follows that

$$\mathcal{F}U(x + m\Delta x, y + n\Delta y, t) = e^{im\xi} e^{in\eta} \hat{U}, \quad (3.63)$$

where

$$\xi \equiv \omega_x \Delta x, \quad \eta \equiv \omega_y \Delta y. \quad (3.64)$$

As in Eq. (3.24), any one step linear finite difference solution to the linear equation Eq. (2.46) may be written

$$\sum_{k,l=-\infty}^{\infty} s_{kl} U_{i+k,j+l}^{n+1} = \sum_{k,l=-\infty}^{\infty} r_{kl} U_{i+k,j+l}^n. \quad (3.65)$$

where the  $s_{kl}$  and  $r_{kl}$  are constants.

We take the Fourier transform of Eq. (3.65) and define the amplification factor  $g(\xi, \eta)$  by

$$\hat{U}^{n+1} = g(\xi, \eta) \hat{U}^n. \quad (3.66)$$

The Von Neumann condition is then

$$|g(\xi, \eta)| \leq 1, \quad -\pi \leq \xi \leq \pi, \quad -\pi \leq \eta \leq \pi. \quad (3.67)$$

### 3.8 The Method of Lines in Two Dimensions

As in the one dimensional case of section 3.6, we write the differential equation in semi-discrete form first,

$$\begin{aligned} \frac{dU_{ij}}{dt} = & -\frac{a}{\Delta x} \delta_x^{(m)} U_{ij} - \frac{b}{\Delta y} \delta_y^{(m)} U_{ij} \\ & + \frac{\kappa}{\Delta x^2} (U_{i+1j} - 2U_{ij} + U_{i-1j}) + \frac{\kappa}{\Delta y^2} (U_{ij+1} - 2U_{ij} + U_{ij-1}), \end{aligned} \quad (3.68)$$

$$\kappa = k \Delta t \frac{c^2}{\sigma}, \quad c = \max(|a|, |b|), \quad (3.69)$$

with  $\sigma$  to be defined below, and then take its Fourier transform to get

$$\frac{d\hat{U}}{dt} = \frac{1}{\Delta t} \Lambda \hat{U}, \quad (3.70)$$

$$\Lambda = -i \frac{a \Delta t}{\Delta x} P^{(m)}(\xi) - i \frac{b \Delta t}{\Delta y} P^{(m)}(\eta) - 4\kappa \frac{\Delta t}{\Delta x^2} \sin^2(\xi/2) - 4\kappa \frac{\Delta t}{\Delta y^2} \sin^2(\eta/2). \quad (3.71)$$

Once again we simply look up the stability region for  $\Lambda$  in the complex plane for the particular time integration method we use. If either method (2.30) or (2.31) is used, we get  $g(\xi, \eta)$  as given by Eq. (3.59), but with  $\Lambda$  as defined above in Eq. (3.71).

Consider now the case of no dissipation ( $\kappa = 0$ ). Then  $\Lambda$  is purely imaginary, and achieves its extreme values for  $\eta = \pm \xi$  such that  $P^{(m)}(\xi)$  is maximized. Since the extreme values of  $\Lambda$  on the imaginary axis for which the method is stable are  $\pm i 2\sqrt{2}$ , we see that

$$\left( \frac{|a|}{\Delta x} + \frac{|b|}{\Delta y} \right) \Delta t P_{\max}^{(m)} \leq 2\sqrt{2}. \quad (3.72)$$

(The absolute value signs are used in (3.72) to cover the case where  $a$  and  $b$  have opposite signs, in which case the most extreme  $\Lambda$  occurs for  $P^{(m)}(\xi)$  and  $P^{(m)}(\eta)$  maximum in magnitude but of opposite sign.) If we *define* the Courant number in two dimensions by

$$\sigma \equiv \left( \frac{|a|}{\Delta x} + \frac{|b|}{\Delta y} \right) \Delta t, \quad (3.73)$$

we recover the familiar stability limit of (3.60), written as

$$\sigma P_{max}^{(m)} \leq 2\sqrt{2}. \quad (3.74)$$

If  $m = 2$ ,  $\sigma \leq 2\sqrt{2}$ ; if  $m = 4$ ,  $\sigma \leq 2.0612$ . We select a stable value for  $\sigma$  and compute  $\Delta t$  from

$$\Delta t = \frac{\sigma}{\frac{|a|}{\Delta x} + \frac{|b|}{\Delta y}}. \quad (3.75)$$

The case where dissipation dominates leads to the result

$$\left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) \kappa \Delta t \leq 0.6963, \quad (3.76)$$

which for  $\kappa$  as defined by Eq. (3.69) puts an upper limit on  $k$  for any given  $\Delta t$ , or vice versa:

$$\left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) \frac{c^2 \Delta t^2}{\sigma} k \leq 0.6963. \quad (3.77)$$

### 3.9 Stability Limits for Fluid Dynamics Problems

As we will see in Chapter 5, the three equations of one dimensional fluid dynamics may be transformed into an equivalent set of coupled nonlinear wave equations. The wave velocities are the characteristic velocities of the system, namely  $v - c$ ,  $v$ , and  $v + c$ , where  $v$  is the fluid velocity, and  $c$  is the speed of sound. It is reasonable to expect that the largest characteristic velocity determines the time step for the whole system. We therefore pick a value for  $\sigma \leq \sigma_{max}$  and compute  $\Delta t$  from

$$\Delta t = \sigma \frac{\Delta x}{\max(c_x)}, \quad (3.78)$$

$$c_x = |v| + c, \quad (3.79)$$

where the maximum is over all points on the grid.

In two dimensions the  $x$  direction characteristic velocities are  $v_x - c$ ,  $v_x$ ,  $v_x + c$ , while the  $y$  direction velocities are  $v_y - c$ ,  $v_y$ ,  $v_y + c$ . Hence we set

$$\Delta t = \frac{\sigma}{\max\left(\frac{c_x}{\Delta x} + \frac{c_y}{\Delta y}\right)}, \quad (3.80)$$

$$c_x = |v_x| + c, \quad c_y = |v_y| + c, \quad (3.81)$$

where the maximum is over all points on the two dimensional grid, and  $\sigma \leq \sigma_{max}$ .

The stability properties of the dissipative terms are essentially the same as in the previous section. A more detailed discussion of dissipation for nonlinear systems will be given in Chapter 4.

### 3.10 Exercises

1. Verify Eq. (3.11) in the one and two dimensional cases, using the explicit solutions for  $u(x, t)$  and  $u(x, y, t)$  given in Chapter 2.
2. Derive Eqs. (3.20)–(3.22).
3. Compute the stability limit for the approximation

$$U_i^{n+1} = U_i^n - \frac{\sigma}{2}(U_i^n - U_{i-2}^n).$$

Could you have predicted this result?

4. Derive Eq. (3.50).
5. Find the real and imaginary intercepts of the equation  $|g(\Lambda)| = 1$ , with  $g$  given by Eq. (3.59), and  $\Lambda$  taken to be a general complex number.

1111 1111 1111



## Chapter 4

# Artificial Viscosity and Conservation Laws

The exercises in Chapter 2 demonstrated the need for artificial viscosity in finite difference approximations which represent discontinuous solutions. The artificial viscosity took the form of added dissipative, or diffusive, terms, which acted to damp numerical oscillations and spread out the discontinuity over a few grid intervals.

One requirement which the added dissipation must satisfy is the consistency condition. The dissipative terms must vanish in the limit as all grid intervals go to zero. Consistency is a necessary condition for valid artificial dissipation, but is far from sufficient. One could define an infinite number of terms which satisfy the consistency condition but which do not have the appropriate behavior.

The purpose of this chapter is to define the "appropriate behavior" for artificial viscosity. However, we must first understand the general properties of the original non-dissipative system, and it is with the system of inviscid fluid dynamics equations that we begin.

### 4.1 Conservation Laws and Tensor Fields

Tensor calculus is the natural language in which to express conservation laws for field quantities because it allows one to write general equations which are coordinate invariant, i.e., which are valid in all coordinate systems. The simpler techniques of vector calculus suffice to describe the conservation of scalar fields, but are inadequate to describe the properties of vector fields. As the momentum density is a conserved vector field, the tensor description will be employed. A brief review of tensor calculus is given in the following sections, but a comprehensive derivation of the formulas is not possible in this text. The interested reader is referred to the book by Weinberg [11], or any text on tensor calculus, for the details.

### 4.1.1 Tensors

A tensor is represented symbolically by a symbol (such as a Greek or Roman letter) followed by some number of upper and lower indices (superscripts and subscripts), as in  $T^{ab}_{cde}$ . The indices may be either letters or numbers. A numerical index refers to a particular tensor component, while a letter index refers to all components, with the understanding that giving the index a numerical value singles out a particular component.

The total number of indices is the *rank* of the tensor. (The above example has a rank of 5.) In a coordinate system with  $n$  dimensions, each index represents a number from 1 to  $n$ <sup>1</sup>, and a tensor of rank  $r$  has  $n^r$  components. For example, the 9 components of the second rank tensor  $A^a_b$  in 3 dimensions are  $A^1_1, A^1_2, A^1_3, A^2_1, A^2_2, A^2_3, A^3_1, A^3_2, A^3_3$ . Tensors of rank zero have no indices, and are called *scalars*. Tensors of rank one have one index, and are usually called *vectors*. Tensors of higher rank have no special names, and are referred to generically as tensors. Tensors of rank two, however, are conveniently written in matrix format, and are sometimes treated as matrices.

Tensors are defined mathematically as objects which satisfy certain coordinate transformation properties. Suppose we have two coordinate systems, one of which has coordinates written as  $x^a = (x^1, x^2, x^3)$ , and the other of which has coordinates  $x^{a'} = (x^1, x^2, x^3)$ . One example of two such systems are the rectangular coordinate system, in which  $x^a = (x, y, z)$ , and the spherical coordinate system, in which  $x^{a'} = (r, \theta, \phi)$ . We can define the following coordinate transformation matrices to relate the two systems:

$$\Lambda^a_{a'} = \frac{\partial x^a}{\partial x^{a'}}, \quad \Lambda^{a'}_a = \frac{\partial x^{a'}}{\partial x^a}. \quad (4.1)$$

A tensor  $T^a_b$  in the unprimed coordinate system may be transformed into an equivalent tensor  $T^{a'}_{b'}$  in the primed system according to

$$T^{a'}_{b'} = \Lambda^{a'}_a \Lambda^b_{b'} T^a_b, \quad (4.2)$$

where repeated indices, with one up and one down, are summed over their range (i.e., 1 to  $n$ ), so that Eq.(4.2) is a compact representation of

$$T^{a'}_{b'} = \sum_{a=1}^n \sum_{b=1}^n \Lambda^{a'}_a \Lambda^b_{b'} T^a_b. \quad (4.3)$$

A tensor with upper indices only is *contravariant*. An example is the coordinate velocity vector  $u^a = dx^a/dt$ , which transforms according to

$$u^{a'} = \frac{dx^{a'}}{dt} = \frac{\partial x^{a'}}{\partial x^a} \frac{dx^a}{dt} = \Lambda^{a'}_a \frac{dx^a}{dt} = \Lambda^{a'}_a u^a. \quad (4.4)$$

A tensor with only lower indices is *covariant*. The gradient  $s_a$  of a scalar  $S$  is covariant, since

$$s_{a'} \equiv \frac{\partial S}{\partial x^{a'}} = \frac{\partial x^a}{\partial x^{a'}} \frac{\partial S}{\partial x^a} = \Lambda^a_{a'} \frac{\partial S}{\partial x^a} = \Lambda^a_{a'} s_a. \quad (4.5)$$

<sup>1</sup>Or 0 to  $n-1$  in general relativity.

The coordinate transformations defined above assume that the origins of the original and transformed systems are the same. Translations (transformations which move the origin) are excluded.<sup>2</sup> The allowed transformations are (1) rotations of a particular coordinate geometry about some axis (e.g., a 45° rotation of a rectangular system about the axis  $x = y = z$ ); (2) transformations from one coordinate geometry to another (e.g., rectangular to spherical); or (3) any combination of (1) and (2).

For example, rectangular and spherical coordinate systems are related by

$$\begin{aligned} x &= r \sin \theta \cos \phi, & r &= \sqrt{x^2 + y^2 + z^2}, \\ y &= r \sin \theta \sin \phi, & \tan \theta &= \frac{\sqrt{x^2 + y^2}}{z}, \\ z &= r \cos \theta, & \tan \phi &= y/x. \end{aligned} \quad (4.6)$$

#### 4.1.2 Coordinate Systems and Metric Tensors

Let  $t$  represent the time coordinate, and  $x^a = (x^1, x^2, x^3)$  represent the spatial coordinates. The vector  $x^a$  is a contravariant vector. The coordinate system denoted by  $x^a$  need not be rectangular coordinates; for example, the choice  $x^a = (r, \phi, z)$  represents cylindrical coordinates, while  $x^a = (r, \theta, \phi)$  represents spherical coordinates. (Note that all indices run from 1 to  $n$ .)

Now consider an object which is moving through our system. At any one time it has spatial coordinates  $x^a$ , but the coordinates change with time. Consequently we may define a *coordinate velocity*  $u^a$  by

$$u^a = \frac{dx^a}{dt}, \quad (4.7)$$

i.e.,  $u^1 = dx^1/dt$ ,  $u^2 = dx^2/dt$ , and  $u^3 = dx^3/dt$ . The coordinate velocity is a contravariant vector whose components are the time derivatives of the spatial coordinates. The coordinate velocity is *not* the same as the *physical velocity*, represented throughout by  $v_a$ , which is the rate of change of distance along the coordinate axes and which is *not* a tensor! For example, the coordinate velocity in spherical coordinates is  $(\dot{r}, \dot{\theta}, \dot{\phi})$ , while the physical velocity components are  $v_r = \dot{r}$ ,  $v_\theta = r\dot{\theta}$ ,  $v_\phi = r \sin \theta \dot{\phi}$ , where the dot denotes derivatives with respect to time.

Clearly we need to relate the coordinate velocity to the more intuitive notion of physical velocity. To do so, we must have some way to relate coordinate changes to the distances spanned by them. In tensor calculus, these two quantities are related by the *metric tensor*  $g_{ab}$ . The metric tensor is a symmetric second rank tensor, whose components are usually functions of the coordinates.

Suppose our test particle moves from position  $x^a = (x^1, x^2, x^3)$  to  $x^a + dx^a = (x^1 + dx^1, x^2 + dx^2, x^3 + dx^3)$ , where  $dx^a$  is a set of small coordinate differentials. In doing so,

<sup>2</sup>The four dimensional spacetime of general relativity involves more general transformations, as time is one of the coordinates to be transformed. *Lorentz transformations* assume coincident origins for the original and transformed spacetime coordinate systems, which means that the spatial origins of the two systems coincide at time  $t = 0$ . *Lorentz boosts* are particular transformations which relate two systems moving with respect to each other, and thus produce time dependent translations.

the particle traverses a distance  $ds$  given by

$$ds^2 = g_{ab} dx^a dx^b. \quad (4.8)$$

The symmetry of the metric tensor implies that only  $n(n+1)/2$  of its  $n^2$  components may be unique (six components in three dimensions). A general metric in three dimensions may be written schematically by a  $3 \times 3$  array of numbers, similar to a matrix,

$$g_{ab} = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix}, \quad (4.9)$$

where by symmetry

$$g_{ab} = g_{ba}. \quad (4.10)$$

In orthogonal coordinate systems, where the coordinate axes are perpendicular to each other, the metric tensor is diagonal, and may be written

$$g_{ab} = \begin{pmatrix} h_1^2 & & \\ & h_2^2 & \\ & & h_3^2 \end{pmatrix}, \quad (4.11)$$

where  $h_1$ ,  $h_2$ , and  $h_3$  are the scale factors for the coordinate directions (and the superscript 2 represents the square of the number, not a tensor index).

A diagonal metric simplifies tensor calculations. For example, we need to know the contravariant (inverse) metric  $g^{ab}$ , defined by

$$g^{ab} g_{bc} = \delta_c^a, \quad g_{ab} g^{bc} = \delta_a^c, \quad (4.12)$$

where  $\delta_a^b$  is the Kronecker delta,

$$\delta_a^b = \begin{cases} 1 & a = b, \\ 0 & a \neq b. \end{cases} \quad (4.13)$$

The inverse of a diagonal metric  $g_{ab}$  is simply

$$g^{ab} = \begin{pmatrix} h_1^{-2} & & \\ & h_2^{-2} & \\ & & h_3^{-2} \end{pmatrix}. \quad (4.14)$$

The inverse of a general tensor is considerably more complicated.

The metric tensor is of crucial importance, not only because it defines the distance relationship for a coordinate system, but because it is also used to transform a contravariant index into a covariant index, and vice-versa, a process referred to as "raising and lowering indices." If  $a$  is a lower index on a tensor, and we wish to raise it, we multiply by  $g^{ab}$  to get a new tensor of the same name with an upper  $b$  index where the old lower  $a$  index was. Similarly, multiplication of a tensor with an upper  $a$  index by  $g_{ab}$  produces a new tensor of the same name with a lower  $b$  index where the old upper  $a$  index was. Some examples are

$$u_b = g_{ab}u^a, \quad u^b = g^{ab}u_b, \quad A_{ab}{}^{cd} = g_{ae}g_{bf}A^{efcd}, \quad (4.15)$$

and so forth.

We can now compute the physical velocity, defined above as the rate of change of distance, per time, in the coordinate directions of an orthogonal coordinate system (described by the diagonal metric of (4.11)). Let the physical velocity have components <sup>3</sup>  $(v_1, v_2, v_3)$ . The distance traversed by a motion which changes the  $j$ th coordinate by  $dx^j$  and does not affect the others is

$$ds = h_j dx^j \quad (\text{not summed}), \quad (4.16)$$

hence

$$v_j = h_j u^j = u_j / h_j \quad (\text{not summed}). \quad (4.17)$$

Thus in spherical coordinates the contravariant (coordinate) velocity  $u^a$  is  $(\dot{r}, \dot{\theta}, \dot{\phi})$ , the covariant velocity  $u_a$  is  $(\dot{r}, r^2 \dot{\theta}, r^2 \sin^2 \theta \dot{\phi})$ , and the physical velocity  $v_a$  is  $(\dot{r}, r \dot{\theta}, r \sin \theta \dot{\phi})$ .

The metrics and inverse metrics for the three most often used coordinate systems are given below.

**Rectangular**  $x^a = (x, y, z)$

$$g_{ab} = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}, \quad g^{ab} = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}, \quad (4.18)$$

**Cylindrical**  $x^a = (r, \phi, z)$

$$g_{ab} = \begin{pmatrix} 1 & & \\ & r^2 & \\ & & 1 \end{pmatrix}, \quad g^{ab} = \begin{pmatrix} 1 & & \\ & r^{-2} & \\ & & 1 \end{pmatrix}, \quad (4.19)$$

---

<sup>3</sup>Remember, the physical velocity is not a tensor!

Spherical  $x^a = (r, \theta, \phi)$

$$g_{ab} = \begin{pmatrix} 1 & & \\ & r^2 & \\ & & r^2 \sin^2 \theta \end{pmatrix}, \quad g^{ab} = \begin{pmatrix} 1 & & \\ & r^{-2} & \\ & & r^{-2} \sin^{-2} \theta \end{pmatrix}. \quad (4.20)$$

### 4.1.3 Combining Tensors

New tensors may be generated from old tensors in a variety of ways. Two tensors of the same type may be added to give a third of that type:

$$A_{bc}^a = B_{bc}^a + C_{bc}^a. \quad (4.21)$$

The product of two tensors of rank  $m$  and  $n$  is a new tensor of rank  $m + n$ ,

$$A_{ab}{}^{cd} = B_{ab} C^{cd}, \quad (4.22)$$

provided no two indices are the same. If two indices (one up, one down) are the same, the implied summation produces a new tensor whose rank is two less than the original, as in

$$R_b^a = S^{ac}{}_{bc}, \quad (4.23)$$

$$T^a{}_{bc} = F^a{}_{de} G_{bc}{}^{de}. \quad (4.24)$$

The summation process is often called contraction, and is a frequent occurrence in tensor calculus. As the number of indices involved increases, the number of terms in the sum increases rapidly. For example, the contraction of a tensor  $R_{abcd}$  with itself to produce a scalar  $R$ , according to

$$R = R_{abcd} R^{abcd}, \quad (4.25)$$

has  $3^4 = 81$  terms in 3 dimensions.<sup>4</sup>

### 4.1.4 Covariant Differentiation

Another way to generate new tensors is to differentiate old ones. The derivative of a tensor with respect to a scalar is a tensor of the same type as the first, as in Eq. (4.7) for the coordinate velocity.<sup>5</sup>

The derivative of a tensor with respect to a coordinate direction is usually *not* a tensor. Such an object is represented either by the usual derivative notation, or by a subscript comma followed by an index indicating the direction of differentiation, as in

$$\frac{\partial f}{\partial x^a} = f_{,a}, \quad \frac{\partial T_{ab}{}^c}{\partial x^e} = T_{ab}{}^c{}_{,e}. \quad (4.26)$$

<sup>4</sup>Such an operation occurs in 4 dimensions in the calculation of tidal forces near black holes, and the corresponding sum has 256 terms!

<sup>5</sup>In relativistic calculations, the time coordinate is part of the four dimensional coordinate vector, not a scalar, and a different definition for velocity is used.

Note that the gradient ( $\partial/\partial x^a$ ) of a scalar is always a tensor (a covariant vector), while gradients of tensors of rank one (vectors) or higher are in general not tensors.

One can define a more general derivative operation than the above which does yield tensor results when applied to a tensor (i.e., which is coordinate invariant). The operator is known as the *covariant derivative* and it reduces to the ordinary derivative of (4.26) when the original tensor is a scalar, or when the coordinate system is rectangular.

The definition of the covariant derivative involves the *connection coefficients*  $\Gamma_{bc}^a$ ,

$$\Gamma_{bc}^a = g^{ad}\Gamma_{dbc}, \quad (4.27)$$

$$\Gamma_{dbc} = \frac{1}{2} \left( \frac{\partial g_{db}}{\partial x^c} + \frac{\partial g_{dc}}{\partial x^b} - \frac{\partial g_{bc}}{\partial x^d} \right). \quad (4.28)$$

Note that  $\Gamma_{bc}^a$  is not itself a tensor, although for computational convenience I have used the metric to raise and lower its first index. The connection coefficients for rectangular, cylindrical, and spherical coordinate systems are given in Appendix A. It is a convenient fact that the connection coefficients for rectangular coordinates are all zero. Note that the coefficients are symmetric on the last two indices ( $\Gamma_{bc}^a = \Gamma_{cb}^a$ ), due to the symmetry of the metric.

The covariant derivative of a tensor in coordinate direction  $a$  is denoted by the subscript ;  $a$ . The following are useful examples:

$$A_{;a} = A_{,a}, \quad (4.29)$$

$$B^a_{;b} = B^a_{,b} + \Gamma_{cb}^a B^c, \quad (4.30)$$

$$B_{a;b} = B_{a,b} - \Gamma_{ab}^c B_c, \quad (4.31)$$

$$C^{ab}_{;c} = C^{ab}_{,c} + \Gamma_{dc}^a C^{db} + \Gamma_{dc}^b C^{ad}, \quad (4.32)$$

$$C^a_{b;c} = C^a_{b,c} + \Gamma_{dc}^a C^d_b - \Gamma_{bc}^d C^a_d, \quad (4.33)$$

$$C_{ab;c} = C_{ab,c} - \Gamma_{ac}^d C_{db} - \Gamma_{bc}^d C_{ad}. \quad (4.34)$$

Covariant derivatives exist for tensors of all ranks, but it will not be necessary to illustrate any more of the possibilities than given above.

One useful property of the definition of covariant differentiation is that the covariant derivative of the metric is always zero:

$$g_{ab;c} = g^{ab}_{;c} = 0. \quad (4.35)$$

Thus the metric commutes with the covariant derivative operator, and we may write expressions such as

$$T^{ab}_{c;e} = (g_{cd}T^{abd})_{;e} = g_{cd}T^{abd}_{;e}. \quad (4.36)$$

Covariant derivatives also obey the usual sum and product rules as ordinary derivatives.

The covariant derivative as defined above adds a single covariant (lower) index to a tensor. We can define a "contravariant derivative" by raising the derivative index with the metric:

$$T^{ab}{}_{;e} \equiv g^{de} T^{ab}{}_{c;d} = (g^{de} T^{ab}{}_c)_{;d}. \quad (4.37)$$

The contraction of a covariant derivative with an index of the original tensor is often called the covariant divergence. Examples of covariant divergence are  $V^a{}_{;a}$ ,  $T^{ab}{}_{;b}$ , and so forth. While the preceding formulas apply just as well to the divergence as to single derivatives, there are some special relations which simplify the divergence calculation.

If we write the metric  $g_{ab}$  as a matrix, then we can compute its determinant. Let

$$g \equiv \sqrt{|\det(g_{ab})|}. \quad (4.38)$$

Then it can be shown that

$$\Gamma^a_{ba} = \frac{1}{g} \frac{\partial g}{\partial x^b} = \frac{\partial}{\partial x^b} \ln g, \quad (4.39)$$

and the divergence of a vector  $V^a$  is

$$V^a{}_{;a} = \frac{1}{g} \frac{\partial}{\partial x^a} (g V^a). \quad (4.40)$$

## 4.2 Fluids as Tensor Fields

Three types of fields are encountered in inviscid fluid dynamics. The density ( $\rho$ ), pressure ( $p$ ), and total energy density ( $e$ ) are scalar fields. The coordinate velocity ( $u^a$ ), momentum density ( $m_a = \rho u_a = \rho g_{ab} u^b$ ), mass flux ( $\rho u^a$ ), and total energy flux ( $[(e + p)u^a]$ ) are vector (first rank tensor) fields. The momentum flux ( $\rho u^a u_b + p \delta^a_b$ ) is a second rank tensor.<sup>6</sup>

The scalar conservation laws for density and total energy are

$$\frac{\partial \rho}{\partial t} + (\rho u^a)_{;a} = 0, \quad (4.41)$$

$$\frac{\partial e}{\partial t} + [(e + p)u^a]_{;a} = 0. \quad (4.42)$$

The momentum equations are more complicated. First we define the (symmetrical) momentum flux tensor [12]

$$T^{ab} = \rho u^a u^b + p g^{ab}, \quad (4.43)$$

or, equivalently,

$$T^b_a = \rho u_a u^b + p \delta^b_a. \quad (4.44)$$

The momentum equations are then

$$\frac{\partial m_a}{\partial t} + T^b_a{}_{;b} = 0, \quad (4.45)$$

<sup>6</sup>If it weren't for the momentum flux, we could get by with the simpler formalism of vector calculus, but such, alas, is not the case.



$$\frac{\partial m_a}{\partial t} + (m_a u^b + p \delta_a^b)_{;b} = 0. \quad (4.46)$$

The system is not complete without the following auxiliary relations. Let  $v$  be the velocity magnitude; then

$$v^2 \equiv u_a u^a = g_{ab} u^a u^b. \quad (4.47)$$

For a perfect gas, the pressure is given by the equation of state

$$p = (\gamma - 1)\epsilon, \quad (4.48)$$

$$\epsilon = e - \frac{1}{2}\rho v^2, \quad (4.49)$$

where  $\epsilon$  is the thermal energy density.

The above equations are useful for formal analysis, but their numerical solution requires writing the equations explicitly in terms of ordinary derivatives. Using the divergence relations of the preceding sections gives the more familiar-looking results:

$$\frac{\partial \rho}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^a} (g \rho u^a) = 0, \quad (4.50)$$

$$\frac{\partial e}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^a} [g(e + p)u^a] = 0, \quad (4.51)$$

$$\frac{\partial m_a}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^b} (g m_a u^b) + \frac{\partial p}{\partial x^a} + \frac{1}{2} \rho u_c u_d \frac{\partial g^{cd}}{\partial x^a} = 0. \quad (4.52)$$

The last term in (4.52) is a "centrifugal force term," which arises in non-rectangular geometries.

Integral forms of the conservation laws may be obtained by multiplying each equation by the volume element  $g dx^1 dx^2 dx^3$  and integrating over the volume desired. If the velocity goes to zero at the boundary of the volume, we get

$$\frac{d}{dt} \int \int_V \int \rho g dx^1 dx^2 dx^3 = 0, \quad (4.53)$$

$$\frac{d}{dt} \int \int_V \int e g dx^1 dx^2 dx^3 = 0, \quad (4.54)$$

and the total mass and energy of the system are constant. The momentum integral is

$$\frac{d}{dt} \int \int_V \int m_a g dx^1 dx^2 dx^3 = - \int \int_V \int \left( \frac{\partial p}{\partial x^a} + \frac{1}{2} \rho u_c u_d \frac{\partial g^{cd}}{\partial x^a} \right) g dx^1 dx^2 dx^3, \quad (4.55)$$

so that the individual components of momentum density are *not* conserved in general, even though the momentum field as a whole is. Note, however, that the rectangular components of momentum density are conserved, since in rectangular coordinates  $g = 1$  and  $\partial g^{cd}/\partial x^a = 0$ , so that

$$\frac{d}{dt} \int \int_V \int m_a g dx^1 dx^2 dx^3 = 0 \quad (\text{rectangular coordinates}) \quad (4.56)$$

assuming  $p$  is constant over the boundary.

The reader who is impatient to see what the complete set of fluid equations looks like may turn to Appendix A, where the equations are written out in full for the three most popular coordinate systems.

### 4.3 Dissipation for Tensor Fields

Let  $\mathbf{U}$  be a generalized density (scalar, vector, or tensor) and  $\mathbf{F} = \mathbf{F}(\mathbf{U})$  be a generalized flux, satisfying the conservation equation

$$\frac{\partial \mathbf{U}}{\partial t} + \text{div}(\mathbf{F}) = 0, \quad (4.57)$$

where  $\text{div}(\mathbf{F})$  is the divergence operator defined in the previous sections. Eq. (4.57) is representative of all the fluid equations.

If the relationship  $\mathbf{F} = \mathbf{F}(\mathbf{U})$  is nonlinear, shock waves are likely to arise in the solution of Eq. (4.57). Even if the flux function is linear, we may still have contact discontinuities in the solution.

Therefore the numerical solution to Eq. (4.57) is likely to require the addition of artificial viscosity, or dissipation, to prevent nonphysical oscillations and nonlinear instabilities in the presence of discontinuities.

The added dissipation must be formulated with care, in such a way as to produce physically meaningful solutions. One could define many dissipative terms which would damp oscillations but introduce nonphysical behavior into the solution.

We add dissipation to the numerical solution by replacing Eq. (4.57) with the equation

$$\frac{\partial \mathbf{U}}{\partial t} + \text{div}(\mathbf{F}) = \mathbf{D}, \quad (4.58)$$

where  $\mathbf{D}$  is the dissipative term. For the presence of  $\mathbf{D}$  in Eq. (4.58) to give meaningful numerical solutions to the *inviscid* Eq. (4.57), we require the following conditions:

1.  $\mathbf{D}$  does not contribute as a source term for conserved fields when integrated over any finite volume, although it may contribute a flux across the boundary of that volume;
2.  $\mathbf{D}$  acts to diffuse (spread out) sharp gradients and damp oscillations;
3.  $\mathbf{D}$  is written in a general form which is valid in all coordinate systems;
4.  $\mathbf{D}$  is isotropic—there are no preferred coordinate directions;
5.  $\mathbf{D}$  vanishes as all grid intervals ( $\Delta t, \Delta x^a$ ) go to zero (consistency condition).

The first point requires that  $\mathbf{D}$  be written as the divergence of some kind of flux. The second point requires that the flux be a diffusive one, involving derivatives of order no higher than first. The third point is satisfied automatically if  $\mathbf{D}$  is written in tensor form. The fourth point requires that the diffusion coefficient which appears in the flux be a scalar, not a tensor of nonzero rank. The fifth point requires that  $\mathbf{D}$  be proportional to some power of a grid interval, and for the fourth point to be satisfied that grid interval must be  $\Delta t$ , and not one of the spatial intervals  $\Delta x^a$ .

In Chapter 2 we found that a monotonic (oscillation free) solution for single wave equations could be obtained by adding to the right side of the equation the term

$$\frac{\partial}{\partial x} \left[ \left( \frac{|\sigma| \Delta x^2}{2 \Delta t} \right) \frac{\partial u}{\partial x} \right],$$

which is a diffusive term with diffusion coefficient  $\frac{|\sigma| \Delta x^2}{2 \Delta t}$ . However, we now require that  $\Delta x$  not appear explicitly in the coefficient, so as to preserve isotropy in the multidimensional case where we will have multiple grid intervals  $\Delta x^a$ . We write  $\mathbf{D}$  as a diffusive term of the form

$$\mathbf{D} = \text{div}[\kappa \text{grad}(\mathbf{U})] \quad (4.59)$$

where  $\kappa$  is a function of position. Eliminating  $\Delta x$  from the above diffusion coefficient in favor of  $\sigma$ ,  $a$ , and  $\Delta t$  gives

$$\kappa = k \Delta t \frac{a^2}{|\sigma|}, \quad (4.60)$$

where  $\sigma$  is the Courant number. This definition will be extended to multidimensional systems in a later section.

### 4.3.1 Scalar Fields

If  $\mathbf{U}$  is a scalar field  $U$ , the flux  $\mathbf{F}$  is a vector with components  $F^a$ , and the conservation equation with dissipation may be written

$$\frac{\partial U}{\partial t} + F^a{}_{;a} = (\kappa U^{;a})_{;a}, \quad (4.61)$$

$$\frac{\partial U}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^a} (g F^a) = \frac{1}{g} \frac{\partial}{\partial x^a} (g \kappa U^{;a}), \quad (4.62)$$

$$\frac{\partial U}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^a} (g F^a) = \frac{1}{g} \frac{\partial}{\partial x^a} \left( g \kappa g^{ab} \frac{\partial U}{\partial x^b} \right). \quad (4.63)$$

### 4.3.2 Vector Fields

If  $\mathbf{U}$  is a covariant vector field<sup>7</sup>  $U_a$ , and the flux  $\mathbf{F}$  is a tensor  $F_a^b$ , the conservation equation with dissipation is

$$\frac{\partial U_a}{\partial t} + F_a^b{}_{;b} = (\kappa U_a^{;b})_{;b}. \quad (4.64)$$

Working out the covariant derivatives on the right and making use of relation (4.39) gives

$$\frac{\partial U_a}{\partial t} + F_a^b{}_{;b} = \frac{1}{g} \frac{\partial}{\partial x^c} \left[ g g^{bc} \kappa \left( \frac{\partial U_a}{\partial x^b} - \Gamma_{ab}^d U_d \right) \right] - \Gamma_{ac}^e \left[ g^{bc} \kappa \left( \frac{\partial U_e}{\partial x^b} - \Gamma_{eb}^d U_d \right) \right]. \quad (4.65)$$

<sup>7</sup>Similar results apply to contravariant vector fields, but the momentum density is most conveniently expressed in terms of covariant fields, so we consider only the covariant case here.

Unfortunately we cannot eliminate the connection coefficients  $\Gamma_{bc}^a$  in favor of simpler expressions, as we did for the scalar equation. The presence of the connection coefficients produces the inhomogeneous term on the right, which implies that the components of  $U_a$  are not conserved in general, except when rectangular coordinates are chosen. In rectangular geometry all  $\Gamma_{bc}^a = 0$ , and we see that the rectangular components of  $U_a$  are conserved. The dissipative operator conserves precisely those components of the field as does the original momentum equation! That the same conservation properties hold in both cases is not an accident, but is a basic property of the geometry of coordinate systems.

## 4.4 More on the Dissipation Coefficient

The fluid equations with dissipation are given in full in Appendix A, and will not be repeated here. Now we will look at the definition of the dissipation coefficient  $\kappa$  in more detail.

As shown in Chapter 2, the choice

$$\kappa = k\Delta t \frac{a^2}{|\sigma|}, \quad \sigma = a(U) \frac{\Delta t}{\Delta x}, \quad (4.66)$$

reproduces the monotone first order scheme of (2.37) when  $k = 1/2$ , but does this definition (and its generalization to higher dimensions) have the conservation, isotropy and coordinate invariance properties we seek?

The answer is a qualified yes. Isotropy can always be maintained by defining  $\kappa$  uniquely at each grid point, so that dissipation occurs at the same “rate” in all coordinate directions. Conservation is guaranteed by the divergence form of the dissipative term, so only coordinate invariance needs to be investigated further.

The definition of  $\kappa$  given above is not coordinate invariant, nor should it be. The dissipation depends on the choice of grid, as it must in order to satisfy the consistency condition, and will change as the grid parameters change. Thus  $\kappa$  is not invariant under grid changes in any given geometry. Moreover, coordinate rotations in multidimensional problems will alter the characteristic velocity components, changing  $a$  and  $\sigma$ , and hence  $\kappa$ . Thus  $\kappa$  is not invariant under coordinate rotations, and is not a scalar.

What happens, then, when we do perform a coordinate transformation on some physical problem and solve the problem numerically in both coordinate systems? Will the two solutions agree? They will, provided both have adequate resolution. By “agree” I do not mean agree exactly (an obvious impossibility, since the two solutions will not even be computed at the same grid points), but the solutions should agree to within 1% or so, except possibly at discontinuities. The diffusion coefficient  $\kappa$  adjusts automatically to changes in the grid and coordinate system so as to apply the correct amount of dissipation needed in each case.

Although strict coordinate invariance is neither necessary nor desirable, strict isotropy is both. If  $\kappa$  is computed differently in the diffusive terms for different coordinate directions, then it is really “simulating” a tensor  $\kappa_b^a$ . For any given problem the results

may appear reasonable. However, to reproduce those results in a new coordinate system would require transforming  $\kappa_b^a$  into  $\kappa_b^{a'} = \Lambda_a^{a'} \Lambda_b^b \kappa_b^a$ , and using  $\kappa_b^{a'}$  in the new system. If the transformation is not performed, the two solutions will in general not agree. If the transformation is performed, the new  $\kappa_b^{a'}$  is likely to contain off diagonal elements and be an explicit function of the transformed coordinates, even though the original  $\kappa_b^a$  was a diagonal tensor with constant elements.

Tensor diffusion coefficients may have a role to play in the real world (such as diffusion and heat conduction in anisotropic materials), but they are of no use in artificial viscosity.

## 4.5 Dissipation in One Dimension

This section illustrates one method for raising the order of the dissipative terms to provide a globally second order accurate solution, for single equations and the one dimensional fluid equations. To get a second order scheme, simply multiply the definition of (4.66) by a function  $\nu(U)$  which is also first order,

$$\kappa = k \Delta t \frac{a^2}{|\sigma|} \nu, \quad (4.67)$$

where  $\nu \approx 1$  in oscillatory regions and near discontinuities, and is a first order quantity otherwise. One definition which has proved quite useful is

$$\nu_i = \frac{|U_{i+1} - 2U_i + U_{i-1}|}{|U_{i+1} - U_i| + |U_i - U_{i-1}|}, \quad (4.68)$$

where  $U_i$  is the numerical solution at grid point  $x_i$ .

In summary, we make a finite difference approximation to the dissipative equation

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = \frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right), \quad f = f(u), \quad (4.69)$$

as in Chapter 2. The semi-discrete approximation is

$$\frac{dU_i}{dt} = -\frac{1}{\Delta x} \delta_x^{(m)} f_i + \frac{1}{\Delta x^2} [\kappa_{i+1/2} (U_{i+1} - U_i) - \kappa_{i-1/2} (U_i - U_{i-1})], \quad (4.70)$$

using the definition (4.67) for  $\kappa$ , where the wave velocity  $a = df/du$ , and the constant  $k$  is constrained by  $k|\sigma| \leq 0.6963$ , for the integration schemes (2.30) and (2.31). (The choice  $k = 0.3$  is often effective.) Note that the quantities  $f$ ,  $\kappa$ ,  $a$ , and  $\sigma = a\Delta t/\Delta x$  are local functions of  $U$  and will generally vary from place to place.

Now consider the more difficult problem of fluid dynamics in one dimension, choosing spherical geometry for the coordinates. Retaining only the radial terms from Eqs. (A.43)–(A.45) gives

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho u^r) = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa \frac{\partial \rho}{\partial r} \right), \quad (4.71)$$

$$\frac{\partial e}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} [r^2(e+p)u^r] = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa \frac{\partial e}{\partial r} \right), \quad (4.72)$$

$$\frac{\partial m_r}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 m_r u^r) + \frac{\partial p}{\partial r} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa \frac{\partial m_r}{\partial r} \right) - \frac{2}{r^2} \kappa m_r, \quad (4.73)$$

where

$$u^r = m_r / \rho, \quad (4.74)$$

$$p = (\gamma - 1) \left( e - \frac{1}{2} \rho u^{r^2} \right) = (\gamma - 1) \left( e - \frac{1}{2} m_r u^r \right), \quad (4.75)$$

and  $\gamma$  is a constant (5/3 for a monatomic gas). Here  $u^r$  is the coordinate velocity, which happens to be the same as the physical velocity  $v_r$  in this case.

The semi-discrete approximation to these equations is

$$\begin{aligned} \frac{d\rho_i}{dt} = & -\frac{1}{r_i^2 \Delta r} \delta_r^{(m)} (r_i^2 \rho_i u_i^r) \\ & + \frac{1}{r_i^2 \Delta r^2} \left[ r_{i+1/2}^2 \kappa_{i+1/2} (\rho_{i+1} - \rho_i) - r_{i-1/2}^2 \kappa_{i-1/2} (\rho_i - \rho_{i-1}) \right], \end{aligned} \quad (4.76)$$

$$\begin{aligned} \frac{de_i}{dt} = & -\frac{1}{r_i^2 \Delta r} \delta_r^{(m)} [r_i^2 (e_i + p_i) u_i^r] \\ & + \frac{1}{r_i^2 \Delta r^2} \left[ r_{i+1/2}^2 \kappa_{i+1/2} (e_{i+1} - e_i) - r_{i-1/2}^2 \kappa_{i-1/2} (e_i - e_{i-1}) \right], \end{aligned} \quad (4.77)$$

$$\begin{aligned} \frac{dm_{ri}}{dt} = & -\frac{1}{r_i^2 \Delta r} \delta_r^{(m)} (r_i^2 m_{ri} u_i^r) - \frac{1}{\Delta r} \delta_r^{(m)} p_i \\ & + \frac{1}{r_i^2 \Delta r^2} \left[ r_{i+1/2}^2 \kappa_{i+1/2} (m_{ri+1} - m_{ri}) - r_{i-1/2}^2 \kappa_{i-1/2} (m_{ri} - m_{ri-1}) \right] \\ & - \frac{2}{r_i^2} \kappa_i m_{ri}. \end{aligned} \quad (4.78)$$

To compute the diffusion coefficients we need to define an effective wave speed  $a$ . In the case of a single equation,  $a$  was just the local value of  $df/du$ . In the current problem we have three equations, and there are three characteristic velocities (as will be shown in Chapter 5). The three characteristic velocities are  $u^r - c$ ,  $u^r$ , and  $u^r + c$ , where  $c = \sqrt{\gamma p / \rho}$  is the speed of sound. The amount of dissipation needed is governed by the most rapidly changing wave. Hence we define the quantity  $c_r$  to be the magnitude of the greatest wave velocity in the  $r$  direction,

$$c_{ri} = |u_i^r| + c_i, \quad (4.79)$$

$$\sigma_i = \Delta t \frac{c_{ri}}{\Delta r}, \quad (4.80)$$

and set

$$a_i = c_{ri}. \quad (4.81)$$

Then the dissipation coefficient is given by

$$\kappa_i = k \Delta t \frac{a_i^2}{|\sigma_i|} \nu_i, \quad \kappa_{i+1/2} = \frac{1}{2} (\kappa_i + \kappa_{i+1}), \quad (4.82)$$

where  $\nu_i$  may be made a function of any solution component ( $\rho$ ,  $m$ ,  $e$ , or some combination). The choice  $\nu = \nu(p)$  has been found to be effective, so we define

$$\nu_i = \frac{|p_{i+1} - 2p_i + p_{i-1}|}{|p_{i+1} - p_i| + |p_i - p_{i-1}|}. \quad (4.83)$$

Note that the equations are undefined at  $r = 0$ , because of the coordinate singularity. The time derivatives become infinite at  $r = 0$  unless  $u^r(r = 0, t) \equiv 0$ , in which case L'Hopital's rule gives

$$\frac{\partial \rho}{\partial t} + 3 \frac{\partial}{\partial r}(\rho u^r) = 3 \frac{\partial}{\partial r} \left( \kappa \frac{\partial \rho}{\partial r} \right) \Big|_{r=0}, \quad (4.84)$$

$$\frac{\partial e}{\partial t} + 3 \frac{\partial}{\partial r}[(e + p)u^r] = 3 \frac{\partial}{\partial r} \left( \kappa \frac{\partial e}{\partial r} \right) \Big|_{r=0}, \quad (4.85)$$

$$m_r = 0 \Big|_{r=0}. \quad (4.86)$$

We know from the condition of spherical symmetry that  $\rho$ ,  $e$ , and  $p$  are symmetric functions of  $r$ , while  $m_r$  and  $u^r$  are antisymmetric, and can use these symmetry conditions to evaluate the finite difference approximations at and near  $r = 0$ .

## 4.6 Dissipation in Two and Three Dimensions

The simplest two dimensional problem is the single conservation law of Eqs. (2.45)–(2.46), to which we add dissipation as follows:

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} = \frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial u}{\partial y} \right). \quad (4.87)$$

The  $x$  direction characteristic velocity is  $a = df/du$ , and the  $y$  direction velocity is  $b = dg/du$ .

The semi-discrete approximation to (4.68) is

$$\begin{aligned} \frac{dU_{ij}}{dt} = & -\frac{1}{\Delta x} \delta_x^{(m)} f_{ij} - \frac{1}{\Delta y} \delta_y^{(m)} g_{ij} \\ & + \frac{1}{\Delta x^2} [\kappa_{i+1/2, j} (U_{i+1, j} - U_{ij}) - \kappa_{i-1/2, j} (U_{ij} - U_{i-1, j})] \\ & + \frac{1}{\Delta y^2} [\kappa_{i, j+1/2} (U_{ij+1} - U_{ij}) - \kappa_{i, j-1/2} (U_{ij} - U_{i, j-1})]. \end{aligned} \quad (4.88)$$

The local Courant number is

$$\sigma_{ij} = \Delta t \left( \frac{|a_{ij}|}{\Delta x} + \frac{|b_{ij}|}{\Delta y} \right). \quad (4.89)$$

Now select the dissipation on the basis of the maximum velocity component,

$$c_{ij} = \max(|a_{ij}|, |b_{ij}|), \quad (4.90)$$

$$\kappa_{ij} = k \Delta t \frac{c_{ij}^2}{\sigma_{ij}} \nu_{ij}, \quad (4.91)$$

$$\kappa_{i+1/2 \ j} = \frac{1}{2}(\kappa_{ij} + \kappa_{i+1 \ j}), \quad \kappa_{ij+1/2} = \frac{1}{2}(\kappa_{ij} + \kappa_{ij+1}), \quad (4.92)$$

where

$$\nu_{ij} = \max \left( \frac{|U_{i+1 \ j} - 2U_{ij} + U_{i-1 \ j}|}{|U_{i+1 \ j} - U_{ij}| + |U_{ij} - U_{i-1 \ j}|}, \frac{|U_{ij+1} - 2U_{ij} + U_{ij-1}|}{|U_{ij+1} - U_{ij}| + |U_{ij} - U_{ij-1}|} \right). \quad (4.93)$$

Finally we consider the fluid equations in three dimensions, and in cylindrical coordinates  $(r, \phi, z)$ . The equations, with dissipation, are

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r \rho u^r) + \frac{\partial}{\partial \phi} (\rho u^\phi) + \frac{\partial}{\partial z} (\rho u^z) \\ = \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa \frac{\partial \rho}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \phi} \left( \kappa \frac{\partial \rho}{\partial \phi} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial \rho}{\partial z} \right), \end{aligned} \quad (4.94)$$

$$\begin{aligned} \frac{\partial e}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} [r(e+p)u^r] + \frac{\partial}{\partial \phi} [(e+p)u^\phi] + \frac{\partial}{\partial z} [(e+p)u^z] \\ = \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa \frac{\partial e}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \phi} \left( \kappa \frac{\partial e}{\partial \phi} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial e}{\partial z} \right), \end{aligned} \quad (4.95)$$

$$\begin{aligned} \frac{\partial m_r}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r m_r u^r) + \frac{\partial}{\partial \phi} (m_r u^\phi) + \frac{\partial}{\partial z} (m_r u^z) + \frac{\partial p}{\partial r} - r \rho u^{\phi 2} \\ = \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa \frac{\partial m_r}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \phi} \left[ \kappa \left( \frac{\partial m_r}{\partial \phi} - \frac{m_\phi}{r} \right) \right] + \frac{\partial}{\partial z} \left( \kappa \frac{\partial m_r}{\partial z} \right) \\ - \frac{1}{r^3} \kappa \left( \frac{\partial m_\phi}{\partial \phi} + r m_r \right), \end{aligned} \quad (4.96)$$

$$\begin{aligned} \frac{\partial m_\phi}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r m_\phi u^r) + \frac{\partial}{\partial \phi} (m_\phi u^\phi) + \frac{\partial}{\partial z} (m_\phi u^z) + \frac{\partial p}{\partial \phi} \\ = \frac{1}{r} \frac{\partial}{\partial r} \left[ r \kappa \left( \frac{\partial m_\phi}{\partial r} - \frac{m_\phi}{r} \right) \right] + \frac{1}{r^2} \frac{\partial}{\partial \phi} \left[ \kappa \left( \frac{\partial m_\phi}{\partial \phi} + r m_r \right) \right] \\ + \frac{\partial}{\partial z} \left( \kappa \frac{\partial m_\phi}{\partial z} \right) + \frac{1}{r} \kappa \left( \frac{\partial m_r}{\partial \phi} - \frac{\partial m_\phi}{\partial r} \right), \end{aligned} \quad (4.97)$$

$$\begin{aligned} \frac{\partial m_z}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r m_z u^r) + \frac{\partial}{\partial \phi} (m_z u^\phi) + \frac{\partial}{\partial z} (m_z u^z) + \frac{\partial p}{\partial z} \\ = \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa \frac{\partial m_z}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \phi} \left( \kappa \frac{\partial m_z}{\partial \phi} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial m_z}{\partial z} \right), \end{aligned} \quad (4.98)$$

where

$$u^r = m_r / \rho, \quad u^\phi = m_\phi / (r^2 \rho), \quad u^z = m_z / \rho, \quad (4.99)$$

$$\begin{aligned} p &= (\gamma - 1) \left[ e - \frac{1}{2} \rho (u^{r2} + r^2 u^{\phi 2} + u^{z2}) \right] \\ &= (\gamma - 1) \left[ e - \frac{1}{2} (m_r u^r + m_\phi u^\phi + m_z u^z) \right], \end{aligned} \quad (4.100)$$



and  $\gamma$  is a constant (5/3 for a monatomic gas). The coordinate velocity  $u^a$  is used in these equations, rather than the physical velocity  $v_a (= h_a u^a$ , not summed), as the equations have a simpler (and less singular) form when coordinate velocities are used. Note that  $m_\phi$  is an angular momentum, not a linear momentum:  $m_\phi = \rho u_\phi = g_{\phi\phi} \rho u^\phi = r^2 \rho \dot{\phi} = r \rho v_\phi$ .

The semi-discrete approximation to these equations at the grid points  $(r_i, \phi_j, z_k)$ , where  $r_i = i\Delta r$ ,  $\phi_j = j\Delta\phi$ ,  $z_k = k\Delta z$ , is then

$$\begin{aligned} \frac{d\rho_{ijk}}{dt} = & -\frac{1}{r_i \Delta r} \delta_r^{(m)}(r_i \rho_{ijk} u_{ijk}^r) - \frac{1}{\Delta\phi} \delta_\phi^{(m)}(\rho_{ijk} u_{ijk}^\phi) - \frac{1}{\Delta z} \delta_z^{(m)}(\rho_{ijk} u_{ijk}^z) \\ & + \frac{1}{r_i \Delta r^2} [r_{i+1/2} \kappa_{i+1/2, jk} (\rho_{i+1, jk} - \rho_{ijk}) - r_{i-1/2} \kappa_{i-1/2, jk} (\rho_{ijk} - \rho_{i-1, jk})] \\ & + \frac{1}{r_i^2 \Delta\phi^2} [\kappa_{ij+1/2, k} (\rho_{ij+1, k} - \rho_{ijk}) - \kappa_{ij-1/2, k} (\rho_{ijk} - \rho_{ij-1, k})] \\ & + \frac{1}{\Delta z^2} [\kappa_{ijk+1/2} (\rho_{ijk+1} - \rho_{ijk}) - \kappa_{ijk-1/2} (\rho_{ijk} - \rho_{ijk-1})], \end{aligned} \quad (4.101)$$

$$\begin{aligned} \frac{de_{ijk}}{dt} = & -\frac{1}{r_i \Delta r} \delta_r^{(m)}[r_i (e_{ijk} + p_{ijk}) u_{ijk}^r] - \frac{1}{\Delta\phi} \delta_\phi^{(m)}[(e_{ijk} + p_{ijk}) u_{ijk}^\phi] \\ & - \frac{1}{\Delta z} \delta_z^{(m)}[(e_{ijk} + p_{ijk}) u_{ijk}^z] \\ & + \frac{1}{r_i \Delta r^2} [r_{i+1/2} \kappa_{i+1/2, jk} (e_{i+1, jk} - e_{ijk}) - r_{i-1/2} \kappa_{i-1/2, jk} (e_{ijk} - e_{i-1, jk})] \\ & + \frac{1}{r_i^2 \Delta\phi^2} [\kappa_{ij+1/2, k} (e_{ij+1, k} - e_{ijk}) - \kappa_{ij-1/2, k} (e_{ijk} - e_{ij-1, k})] \\ & + \frac{1}{\Delta z^2} [\kappa_{ijk+1/2} (e_{ijk+1} - e_{ijk}) - \kappa_{ijk-1/2} (e_{ijk} - e_{ijk-1})], \end{aligned} \quad (4.102)$$

$$\begin{aligned} \frac{dm_{r,ijk}}{dt} = & -\frac{1}{r_i \Delta r} \delta_r^{(m)}(r_i m_{r,ijk} u_{ijk}^r) - \frac{1}{\Delta\phi} \delta_\phi^{(m)}(m_{r,ijk} u_{ijk}^\phi) - \frac{1}{\Delta z} \delta_z^{(m)}(m_{r,ijk} u_{ijk}^z) \\ & - \frac{1}{\Delta r} \delta_r^{(m)} p_{ijk} + r_i \rho_{ijk} u_{ijk}^{\phi 2} \\ & + \frac{1}{r_i \Delta r^2} [r_{i+1/2} \kappa_{i+1/2, jk} (m_{r, i+1, jk} - m_{r,ijk}) - r_{i-1/2} \kappa_{i-1/2, jk} (m_{r,ijk} - m_{r, i-1, jk})] \\ & + \frac{1}{r_i^2 \Delta\phi} \left[ \kappa_{ij+1/2, k} \left( \frac{m_{r, ij+1, k} - m_{r,ijk}}{\Delta\phi} - \frac{m_{\phi, ij+1, k} + m_{\phi,ijk}}{2r_i} \right) \right. \\ & \left. - \kappa_{ij-1/2, k} \left( \frac{m_{r,ijk} - m_{r, ij-1, k}}{\Delta\phi} - \frac{m_{\phi,ijk} + m_{\phi, ij-1, k}}{2r_i} \right) \right] \\ & + \frac{1}{\Delta z^2} [\kappa_{ijk+1/2} (m_{r,ijk+1} - m_{r,ijk}) - \kappa_{ijk-1/2} (m_{r,ijk} - m_{r,ijk-1})] \\ & - \frac{1}{r_i^3} \kappa_{ijk} \left( \frac{m_{\phi, ij+1, k} - m_{\phi, ij-1, k}}{2\Delta\phi} + r_i m_{r,ijk} \right), \end{aligned} \quad (4.103)$$

$$\begin{aligned}
\frac{dm_{\phi\ ijk}}{dt} = & -\frac{1}{r_i\Delta r}\delta_r^{(m)}(r_i m_{\phi\ ijk} u_{ijk}^r) - \frac{1}{\Delta\phi}\delta_\phi^{(m)}(m_{\phi\ ijk} u_{ijk}^\phi) - \frac{1}{\Delta z}\delta_z^{(m)}(m_{\phi\ ijk} u_{ijk}^z) \\
& - \frac{1}{\Delta\phi}\delta_\phi^{(m)} p_{ijk} \\
& + \frac{1}{r_i\Delta r} \left[ r_{i+1/2}\kappa_{i+1/2\ jk} \left( \frac{m_{\phi\ i+1\ jk} - m_{\phi\ ijk}}{\Delta r} - \frac{m_{\phi\ i+1\ jk} + m_{\phi\ ijk}}{2r_{i+1/2}} \right) \right. \\
& \left. - r_{i-1/2}\kappa_{i-1/2\ jk} \left( \frac{m_{\phi\ ijk} - m_{\phi\ i-1\ jk}}{\Delta r} - \frac{m_{\phi\ ijk} + m_{\phi\ i-1\ jk}}{2r_{i-1/2}} \right) \right] \\
& + \frac{1}{r_i^2\Delta\phi} \left[ \kappa_{ij+1/2\ k} \left( \frac{m_{\phi\ ij+1\ k} - m_{\phi\ ijk}}{\Delta\phi} + r_i \frac{m_{r\ ij+1\ k} + m_{r\ ijk}}{2} \right) \right. \\
& \left. - \kappa_{ij-1/2\ k} \left( \frac{m_{\phi\ ijk} - m_{\phi\ ij-1\ k}}{\Delta\phi} + r_i \frac{m_{r\ ijk} + m_{r\ ij-1\ k}}{2} \right) \right] \\
& + \frac{1}{\Delta z^2} \left[ \kappa_{ijk+1/2} (m_{\phi\ ijk+1} - m_{\phi\ ijk}) - \kappa_{ijk-1/2} (m_{\phi\ ijk} - m_{\phi\ ijk-1}) \right] \\
& + \frac{1}{r_i} \kappa_{ijk} \left( \frac{m_{r\ ij+1\ k} - m_{r\ ij-1\ k}}{2\Delta\phi} - \frac{m_{\phi\ i+1\ jk} - m_{\phi\ i-1\ jk}}{2\Delta r} \right), \tag{4.104}
\end{aligned}$$

$$\begin{aligned}
\frac{dm_{z\ ijk}}{dt} = & -\frac{1}{r_i\Delta r}\delta_r^{(m)}(r_i m_{z\ ijk} u_{ijk}^r) - \frac{1}{\Delta\phi}\delta_\phi^{(m)}(m_{z\ ijk} u_{ijk}^\phi) - \frac{1}{\Delta z}\delta_z^{(m)}(m_{z\ ijk} u_{ijk}^z) \\
& - \frac{1}{\Delta z}\delta_z^{(m)} p_{ijk} \\
& + \frac{1}{r_i\Delta r^2} \left[ r_{i+1/2}\kappa_{i+1/2\ jk} (m_{z\ i+1\ jk} - m_{z\ ijk}) - r_{i-1/2}\kappa_{i-1/2\ jk} (m_{z\ ijk} - m_{z\ i-1\ jk}) \right] \\
& + \frac{1}{r_i^2\Delta\phi^2} \left[ \kappa_{ij+1/2\ k} (m_{z\ ij+1\ k} - m_{z\ ijk}) - \kappa_{ij-1/2\ k} (m_{z\ ijk} - m_{z\ ij-1\ k}) \right] \\
& + \frac{1}{\Delta z^2} \left[ \kappa_{ijk+1/2} (m_{z\ ijk+1} - m_{z\ ijk}) - \kappa_{ijk-1/2} (m_{z\ ijk} - m_{z\ ijk-1}) \right]. \tag{4.105}
\end{aligned}$$

This system has the characteristic velocity components  $u^r - c$ ,  $u^r$ ,  $u^r + c$  in the  $r$  direction;  $r u^\phi - c$ ,  $r u^\phi$ ,  $r u^\phi + c$  in the  $\phi$  direction; and  $u^z - c$ ,  $u^z$ , and  $u^z + c$  in the  $z$  direction, where  $c = \sqrt{\gamma p/\rho}$  is the speed of sound. To compute the dissipation, we first define the largest characteristic velocity magnitude in each direction according to

$$c_r = |u^r| + c, \quad c_\phi = |r u^\phi| + c, \quad c_z = |u^z| + c; \tag{4.106}$$

define the Courant number as

$$\sigma = \Delta t \left( \frac{c_r}{\Delta r} + \frac{c_\phi}{r\Delta\phi} + \frac{c_z}{\Delta z} \right); \tag{4.107}$$

and select the largest of the three values in (4.106) as the effective velocity  $a$ :

$$a = \max(c_r, c_\phi, c_z). \tag{4.108}$$

The dissipation coefficient is then

$$\kappa_{ijk} = k \Delta t \frac{a_{ijk}^2}{\sigma_{ijk}} \nu_{ijk}, \quad (4.109)$$

where  $\nu_{ijk}$  is taken to be

$$\nu_{ijk} = \max \left( \frac{|p_{i+1 \ jk} - 2p_{ijk} + p_{i-1 \ jk}|}{|p_{i+1 \ jk} - p_{ijk}| + |p_{ijk} - p_{i-1 \ jk}|}, \frac{|p_{ij+1 \ k} - 2p_{ijk} + p_{ij-1 \ k}|}{|p_{ij+1 \ k} - p_{ijk}| + |p_{ijk} - p_{ij-1 \ k}|}, \frac{|p_{ijk+1} - 2p_{ijk} + p_{ijk-1}|}{|p_{ijk+1} - p_{ijk}| + |p_{ijk} - p_{ijk-1}|} \right), \quad (4.110)$$

where  $p$  is the pressure. As usual, the dissipation coefficients at the half points are given by

$$\kappa_{i+1/2 \ jk} = \frac{1}{2}(\kappa_{ijk} + \kappa_{i+1 \ jk}), \quad \kappa_{ij+1/2 \ k} = \frac{1}{2}(\kappa_{ijk} + \kappa_{ij+1 \ k}), \quad \kappa_{ijk+1/2} = \frac{1}{2}(\kappa_{ijk} + \kappa_{ijk+1}). \quad (4.111)$$

## 4.7 Coordinate Singularities

The fluid equations given above for cylindrical coordinates contain a coordinate singularity at  $r = 0$ . In the one dimensional spherical case we dealt with the singularity at  $r = 0$  by requiring that the divergence term in each equation be finite, which allowed us to use L'Hopital's rule to get a non-singular limiting form at the origin. We generally cannot require that each divergence term in an equation be finite at a singularity when dealing with two or three dimensional problems, as it is only necessary that the *sum* of all divergence terms be finite. (This problem becomes particularly acute in spherical coordinates, which is singular at  $r = 0$  for all  $\theta$  values, and at  $\theta = 0, \theta = \pi$  for all  $r$  values.) It is quite possible that any given term may tend to infinity as at the singularity, even though the sum of all such terms in the equation is finite.

The completely general three dimensional problem in non-rectangular coordinates is probably best handled by reverting to the rectangular coordinate definition for the divergence at the singular points, if individual terms are known to become infinite. If on the other hand particular symmetries of the problem dictate that individual terms remain finite at singularities, then L'Hopital's rule may be used to obtain a limiting form for the equations.

## 4.8 Dissipation for General Hyperbolic Problems

So far we have looked only at the fluid dynamics equations. However, the formalism used above may be stated in very general terms for any first order system of hyperbolic conservation laws, in any number of spatial dimensions. In this section I will describe how to construct dissipative terms for an arbitrary system in three spatial dimensions,

representing conservation laws for conserved scalar and covariant vector fields. The reader who is interested in less (or more!) than three dimensions should have no trouble making the appropriate changes.

Our system will have  $l$  conservation equations for the scalar densities  $\alpha_{(1)}, \alpha_{(2)}, \dots, \alpha_{(l)}$ , involving  $l$  flux vectors  $f_{(1)}^a, f_{(2)}^a, \dots, f_{(l)}^a$ , where the subscripts are names for the different densities, not tensor indices.<sup>8</sup> The equations are of the form

$$\frac{\partial \alpha_{(i)}}{\partial t} + f_{(i)}^a{}_{;a} = 0. \quad (4.112)$$

We also have  $m$  conservation laws for the covariant vector densities  $\beta_{(1)a}, \beta_{(2)a}, \dots, \beta_{(m)a}$ , involving  $m$  flux tensors  $F_{(1)a}{}^b, F_{(2)a}{}^b, \dots, F_{(m)a}{}^b$ .<sup>9</sup> Note that tensor indices run from 1 to 3, so there are  $3m$  such equations, of the form

$$\frac{\partial \beta_{(i)a}}{\partial t} + F_{(i)a}{}^b{}_{;b} = 0. \quad (4.113)$$

Using the definitions for covariant derivatives gives the scalar equations as

$$\frac{\partial \alpha_{(i)}}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^a} (g f_{(i)}^a) = 0, \quad i = 1, \dots, l, \quad (4.114)$$

and the vector equations as

$$\frac{\partial \beta_{(i)a}}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^b} (g F_{(i)a}{}^b) - \Gamma_{ab}^c F_{(i)c}{}^b = 0, \quad a = 1, 2, 3, \quad i = 1, \dots, m. \quad (4.115)$$

The total number of differential equations is  $n = l + 3m$ . (There may be, and usually are, some number of algebraic equations required to close the system, such as the equation of state.) It is convenient to define a single unknown variable vector  $\mathbf{U}$  and the three associated flux vectors  $\mathbf{F}_a$  by

$$\mathbf{U} = \begin{pmatrix} \alpha_{(1)} \\ \dots \\ \alpha_{(l)} \\ \beta_{(1)1} \\ \beta_{(1)2} \\ \beta_{(1)3} \\ \dots \\ \beta_{(m)1} \\ \beta_{(m)2} \\ \beta_{(m)3} \end{pmatrix}, \quad \mathbf{F}_a = \begin{pmatrix} f_{(1)}^a \\ \dots \\ f_{(l)}^a \\ F_{(1)1}^a \\ F_{(1)2}^a \\ F_{(1)3}^a \\ \dots \\ F_{(m)1}^a \\ F_{(m)2}^a \\ F_{(m)3}^a \end{pmatrix}, \quad (4.116)$$

<sup>8</sup>For the fluid problems discussed so far,  $l = 2$ ,

$\alpha_{(1)} = \rho$  and  $\alpha_{(2)} = e$ .

<sup>9</sup>The fluid problem has  $m = 1$ , with  $\beta_{(1)a} = m_a$ .

so that the complete set of conservation laws may be written

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}_1}{\partial x^1} + \frac{\partial \mathbf{F}_2}{\partial x^2} + \frac{\partial \mathbf{F}_3}{\partial x^3} + \mathbf{D} = 0, \quad (4.117)$$

where  $\mathbf{D}$  is a vector of inhomogeneous terms. (By vector in this instance I mean any set of variables in the sense of linear algebra, not a tensor. The objects  $\mathbf{U}$ ,  $\mathbf{F}_a$ , and  $\mathbf{D}$  do not satisfy tensor coordinate transformations.)

The equations may also be written

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{U}}{\partial x^1} + \mathbf{B} \frac{\partial \mathbf{U}}{\partial x^2} + \mathbf{C} \frac{\partial \mathbf{U}}{\partial x^3} + \mathbf{D} = 0, \quad (4.118)$$

where  $\mathbf{A}$ ,  $\mathbf{B}$ , and  $\mathbf{C}$  are the  $n \times n$  Jacobian coefficient matrices with components

$$A_{ij} = \frac{\partial F_{1i}}{\partial U_j}, \quad B_{ij} = \frac{\partial F_{2i}}{\partial U_j}, \quad C_{ij} = \frac{\partial F_{3i}}{\partial U_j}. \quad (4.119)$$

Now let the eigenvalues of  $\mathbf{A}$ ,  $\mathbf{B}$ , and  $\mathbf{C}$  be  $\lambda_i$ ,  $\mu_i$ , and  $\eta_i$ ,  $i = 1, \dots, n$ . These eigenvalues are the characteristic velocity components for the associated coordinate directions:  $\lambda_i$  for the  $x^1$  direction,  $\mu_i$  for the  $x^2$  direction, and  $\eta_i$  for the  $x^3$  direction. The extreme values are

$$c_1 = \max |\lambda_i|, \quad c_2 = \max |\mu_i|, \quad c_3 = \max |\eta_i|, \quad (4.120)$$

and the largest of these is

$$a = \max(c_1, c_2, c_3). \quad (4.121)$$

The dissipation coefficient is therefore

$$\kappa = k \Delta t \frac{a^2}{\sigma}, \quad (4.122)$$

where the Courant number is

$$\sigma = \Delta t \left( \frac{c_1}{\Delta x^1} + \frac{c_2}{\Delta x^2} + \frac{c_3}{\Delta x^3} \right). \quad (4.123)$$

The quantity  $\nu$  at grid point  $(x_i^1, x_j^2, x_k^3)$  is then

$$\nu_{ijk} = \max \left( \frac{|f_{i+1jk} - 2f_{ijk} + f_{i-1jk}|}{|f_{i+1jk} - f_{ijk}| + |f_{ijk} - f_{i-1jk}|}, \frac{|f_{ij+1k} - 2f_{ijk} + f_{ij-1k}|}{|f_{ij+1k} - f_{ijk}| + |f_{ijk} - f_{ij-1k}|}, \frac{|f_{ijk+1} - 2f_{ijk} + f_{ijk-1}|}{|f_{ijk+1} - f_{ijk}| + |f_{ijk} - f_{ijk-1}|} \right), \quad (4.124)$$

where  $f$  is any scalar variable which reliably indicates the presence of discontinuities and oscillations, such as pressure in the fluid case.

The equations with dissipation are then

$$\frac{\partial \alpha_{(i)}}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^a} (g f_{(i)}^a) = \frac{1}{g} \frac{\partial}{\partial x^a} \left( g \kappa g^{ab} \frac{\partial \alpha_{(i)}}{\partial x^b} \right) \quad (4.125)$$

for the scalar fields, and

$$\begin{aligned} \frac{\partial \beta_{(i)a}}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^b} (g F_{(i)a}{}^b) - \Gamma_{ab}^c F_{(i)c}{}^b \\ = \frac{1}{g} \frac{\partial}{\partial x^c} \left[ g \kappa g^{bc} \left( \frac{\partial \beta_{(i)a}}{\partial x^b} - \Gamma_{ab}^d \beta_{(i)d} \right) \right] - \Gamma_{ac}^e \kappa g^{bc} \left( \frac{\partial \beta_{(i)e}}{\partial x^b} - \Gamma_{eb}^d \beta_{(i)d} \right) \end{aligned} \quad (4.126)$$

for the vector fields, as in Eqs. (4.63) and (4.65). The approximation to semi-discrete form is handled as in the previous sections.

## 4.9 Conservation Properties of Finite Difference Equations

The fluid equations may be written in a variety of forms, such as the conservative forms described in this chapter, and the characteristic and primitive forms given in Chapter 5. Finite difference approximations may be made to the equations in any form, with the same formal accuracy, yet all approximations in this text have been made to the conservative forms. The reader may wonder if there is an advantage to be had in using the conservative form in numerical work. The answer is yes.

First of all, the artificial viscosity terms require the conservative equations for their definition. However, once the terms are defined, one could write the equations in another form, so the necessity for artificial viscosity does not *require* that the numerical approximations be in conservative form, though they are more simply written in that form.

More important is the notion of *numerical conservation laws*. The numerical approximation to the conservative equations possesses an exact conservation law which is analogous to the original conservation law embodied by the differential equations, and it is for this reason that the conservative form is preferred in numerical work.

A field  $u$  is said to be conserved if it satisfies the equation

$$\frac{\partial u}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^i} (g f^i) = 0, \quad (4.127)$$

where  $f^i$  is the flux of  $u$  in the  $i$ th coordinate direction. The conservation property is seen most clearly by integrating Eq. (4.127) over the volume  $a^1 \leq x^1 \leq b^1$ ,  $a^2 \leq x^2 \leq b^2$ ,  $a^3 \leq x^3 \leq b^3$ :

$$\int \int_V g dx^1 dx^2 dx^3 \left[ \frac{\partial u}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^i} (g f^i) \right] = 0, \quad (4.128)$$

$$\begin{aligned} \frac{d}{dt} \int \int_V u g dx^1 dx^2 dx^3 = - \int_{a^3}^{b^3} \int_{a^2}^{b^2} (g f^1) \Big|_{a^1}^{b^1} dx^2 dx^3 \\ - \int_{a^3}^{b^3} \int_{a^1}^{b^1} (g f^2) \Big|_{a^2}^{b^2} dx^1 dx^3 - \int_{a^2}^{b^2} \int_{a^1}^{b^1} (g f^3) \Big|_{a^3}^{b^3} dx^1 dx^2. \end{aligned} \quad (4.129)$$

The rate of change of the volume integral of  $u$  is given by the integral of the fluxes over the surface bounding that volume.

A properly chosen numerical approximation to Eq. (4.127) retains an analogous conservation property [13]. If the semi-discrete approximation is written as

$$\begin{aligned} \frac{dU_{ijk}}{dt} + \frac{1}{g_{ijk}} \frac{F_{i+1/2, jk}^1 - F_{i-1/2, jk}^1}{\Delta x^1} + \frac{1}{g_{ijk}} \frac{F_{ij+1/2, k}^2 - F_{ij-1/2, k}^2}{\Delta x^2} \\ + \frac{1}{g_{ijk}} \frac{F_{ijk+1/2}^3 - F_{ijk-1/2}^3}{\Delta x^3} = 0, \end{aligned} \quad (4.130)$$

where  $F^l = g f^l$ , then its summation over the volume elements  $g_{ijk} \Delta x^1 \Delta x^2 \Delta x^3$  gives

$$\begin{aligned} \frac{d}{dt} \sum_{i,j,k=1}^{I,J,K} U_{ijk} g_{ijk} \Delta x^1 \Delta x^2 \Delta x^3 = - \sum_{j,k=1}^{J,K} (F_{i+1/2, jk}^1 - F_{i-1/2, jk}^1) \Delta x^2 \Delta x^3 \\ - \sum_{i,k=1}^{I,K} (F_{ij+1/2, k}^2 - F_{ij-1/2, k}^2) \Delta x^1 \Delta x^3 - \sum_{i,j=1}^{I,J} (F_{ijk+1/2}^3 - F_{ijk-1/2}^3) \Delta x^1 \Delta x^2. \end{aligned} \quad (4.131)$$

The interior fluxes cancel out of the sums, leaving only the sums of normal fluxes over the boundary surface. The numerical scheme of (4.130) yields an exact numerical conservation law. A numerical approximation to a nonconservative equation does not produce a conserved numerical solution.

Eq. (4.130) makes use of finite difference approximations of the form

$$\frac{\partial F}{\partial x} = \frac{F_{i+1/2} - F_{i-1/2}}{\Delta x}, \quad (4.132)$$

which involve *mid-point* fluxes  $F_{i+1/2}$ , rather than grid point fluxes  $F_i$ . The dissipative terms naturally have mid-point fluxes, since the dissipative flux is  $F = g\kappa \partial u / \partial x$ , for which

$$F_{i+1/2} = g_{i+1/2} \kappa_{i+1/2} \frac{U_{i+1} - U_i}{\Delta x} \quad (4.133)$$

to second order in  $\Delta x$ . The convective terms have grid point fluxes  $F_i = g_i f_i$ , however, from which the mid-point fluxes  $F_{i+1/2}$  must be constructed for the proof above to hold. The choice

$$F_{i+1/2} = \frac{1}{2}(F_{i+1} + F_i) \quad (4.134)$$

recovers the familiar second order result, while

$$F_{i+1/2} = \frac{7}{12}(F_{i+1} + F_i) - \frac{1}{12}(F_{i+2} + F_{i-1}) \quad (4.135)$$

recovers the fourth order result. Zalesak [14] gives flux expressions up through eighth order.

Note that it is not necessary to compute  $F_{i+1/2}$  explicitly, as given above, to ensure numerical conservation. The finite difference formulas previously used are properly conservative, as demonstrated by the existence of mid-point fluxes such as (4.133), (4.134), and (4.135), along with the numerical conservation law (4.131).

For example, consider the single equation

$$\frac{\partial u}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x}(gf) = \frac{1}{g} \frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right), \quad (4.136)$$

where  $\kappa$  is the artificial dissipation coefficient. The standard semi-discrete approximation, using a fourth order formula for the convective flux, is

$$\begin{aligned} \frac{dU_i}{dt} = & -\frac{1}{g_i} \frac{1}{12\Delta x} [8(g_{i+1}f_{i+1} - g_{i-1}f_{i-1}) - (g_{i+2}f_{i+2} - g_{i-2}f_{i-2})] \\ & + \frac{1}{g_i} \frac{1}{\Delta x^2} [\kappa_{i+1/2}(U_{i+1} - U_i) - \kappa_{i-1/2}(U_i - U_{i-1})], \end{aligned} \quad (4.137)$$

which is exactly equivalent to

$$\frac{dU_i}{dt} = -\frac{F_{i+1/2} - F_{i-1/2}}{\Delta x}, \quad (4.138)$$

where

$$F_{i+1/2} = \frac{7}{12}(g_{i+1}f_{i+1} + g_i f_i) - \frac{1}{12}(g_{i+2}f_{i+2} + g_{i-1}f_{i-1}) - \kappa_{i+1/2} \frac{U_{i+1} - U_i}{\Delta x}, \quad (4.139)$$

and is therefore numerically conservative.

## 4.10 Test Problems

We now have at our disposal all the tools needed to obtain the numerical solution of some typical fluid dynamics problems. For the sake of simplicity, we consider only one dimensional problems for which the boundary values may be held constant with time, postponing the discussion of nontrivial boundary conditions until Chapter 5. Both rectangular and spherical geometries will be considered, with spatial coordinates  $x$  and  $r$ , respectively.

These one dimensional test problems are evaluated on a grid of unit length, divided into 100 subintervals ( $I = 100$ ,  $\Delta x = \Delta r = 0.01$ ). The value of  $\gamma$  in the equation of state is 5/3 throughout. The figures show the analytical solutions (solid lines) and numerical solutions (dots) for the density  $\rho$ , the pressure  $p$ , the momentum density  $m$ , and the velocity  $v$ , at a time  $t$ . The Courant number  $\sigma$ ,

$$\sigma = \frac{c_x \Delta t}{\Delta x}, \quad (4.140)$$

is set to 1 throughout, where  $c_x = \max(|v_x| + c)$  over the grid (and similarly for  $c_r$ ).

The first example is the shock tube problem, frequently used as a test for hydrodynamical codes (as in Sod [24]), and whose solution is given by Thompson [25]. At time  $t = 0$  the system consists of two spatially constant, stationary states, adjoining at  $x = 0$ . The left state ( $x < 0$ ) has  $\rho = p = 1$ , while the right state has  $\rho = 0.125$ ,  $p = 0.1$ .



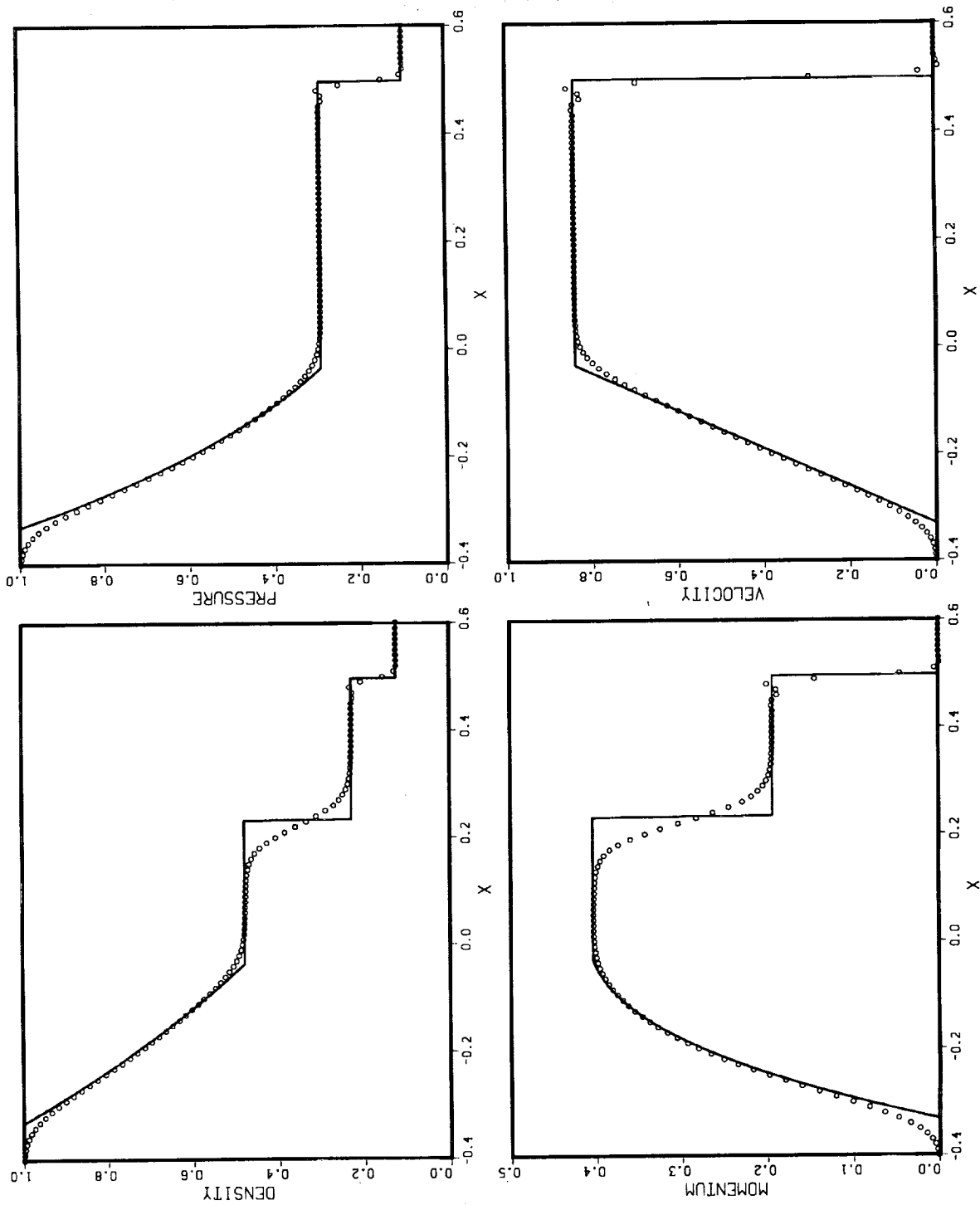


Figure 4.1: Shock tube at step 60

As time progresses, a rarefaction wave forms and moves to the left, while the contact discontinuity and a shock wave move to the right.

Figure 4.1 shows the solution at time step 60,  $t = 0.265$ , with  $k = 0.3$ , just before any waves reach the boundaries.

The shock wave is located at  $x = 0.5$  and is resolved in  $\approx 3$  grid intervals. Small oscillations occur around the shock. These oscillations could be eliminated by increasing  $k$ , at the expense of spreading out the shock (and other features in the solution). The contact discontinuity at  $x = 0.23$  is spread out over  $\approx 10$  grid intervals. Unlike shock waves, which keep a constant width, contact discontinuities in the numerical solution widen steadily with time. The nonlinear nature of the shock wave produces a tendency to steepen which is countered by the artificial viscosity, so the shock width remains constant. However, the contact discontinuity is a discontinuity in a linear wave, which has no steepening tendencies, and therefore spreads monotonically with time as it is diffused by the artificial viscosity.

A general technique for obtaining sharply resolved contact discontinuities has yet to be formulated, and it is beyond the scope of this text to describe any of the numerous experimental methods which have been developed. As a first attempt, one may attempt to detect the presence of such a discontinuity and decrease the artificial viscosity there to reduce the spreading rate. However, some viscosity is needed to prevent oscillations near the contact discontinuity, so the spreading cannot be eliminated by this technique, although it can be slowed. It should also be mentioned that such discontinuities will spread even in the absence of artificial viscosity, as well as producing oscillations.

The next problem considered is the Sedov solution for a spherically symmetric explosion, described by Landau and Lifshitz [12]. (N.B. Eq. (99.10) of the reference should have  $\nu_5 = 2/(\gamma - 2)$ .) An amount of energy  $E$  is deposited at the origin at time  $t = 0$ . The resultant explosion produces a self similar solution bounded by an outgoing spherical shock wave. The density and pressure curves are sharply peaked at the shock, falling off rapidly for decreasing  $r$ . The density goes to zero at the origin, while the pressure flattens out and becomes constant with  $r$  away from the shock. The velocity is linear near the origin, but steepens somewhat near the shock. The similarity solution is valid as long as the shock is very strong, so that the density jump across the shock achieves its maximum value.

The numerical solution is produced by distributing an amount of energy  $E = 1$  over the innermost five grid intervals, in the form of thermal energy. Let the sum of the volume elements for the first five points be

$$vol = 4\pi\Delta r \sum_{i=0}^5 r_i^2, \quad (4.141)$$

then the initial pressure is

$$p_i = (\gamma - 1)E/vol, \quad (4.142)$$

for  $i = 0, \dots, 5$ . For  $i > 5$ ,  $p_i = 10^{-6}$ . We also have  $\rho = 1$  and  $u = 0$  everywhere. The resultant numerical solution is shown in Figure 4.2 at step 365,  $t = 0.614$ , and with  $k = 0.35$ .

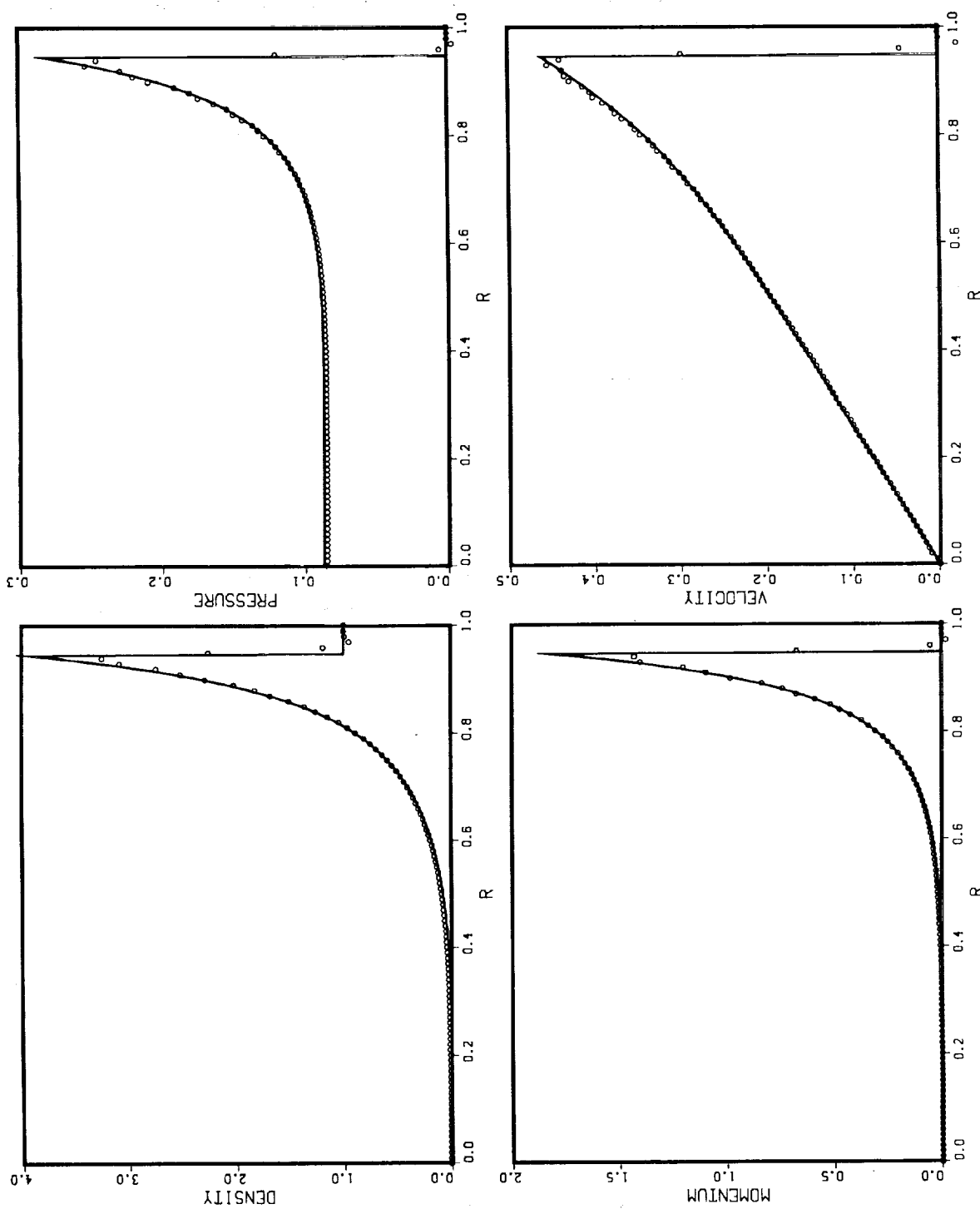


Figure 4.2: Spherical explosion at step 365

The shock wave is very strong, and is resolved in two grid intervals. Once again a small amount of ringing is observed near the shock, which could be eliminated by increasing  $k$  at the expense of spreading out the shock further. The post-shock density should peak exactly at a value of 4 for this problem; the numerical post-shock density is  $\approx 3.25$ , which is low by  $\approx 20\%$ . The density profile behind the shock is so sharply peaked that the numerical solution cannot change quickly enough to achieve the correct density peak. Increasing the resolution of the calculation by increasing the number of grid points would reduce the error in the peak height. However, the correct shock velocity is achieved even though the exact post-shock solution is not attained.

The exact solution to the spherical blast wave has the density going to zero at the origin, while the pressure remains finite and the temperature goes to infinity. The numerical solution cannot reproduce this singular behavior at the origin. Instead the numerical solution has a very small but nonzero density in the center, and a high but finite temperature. The pressure near the center is accurately represented. Note that the sound speed is therefore very large at the center, and is in fact the largest velocity present in the calculation. The allowed time step is therefore determined by the speed of sound at the center, and not by the post-shock velocity, which is much smaller.

## 4.11 Exercises

1. Let  $x^a = (x, y, z)$  be rectangular coordinates, and let  $x^{a'} = (r, \theta, \phi)$  be spherical coordinates. Using the relationships of Eqs. (4.6), compute the transformations  $\Lambda_a^{a'}$  and  $\Lambda_{a'}^a$ .
2. Using the results of problem 1, write down the coordinate velocities  $u^a = (\dot{x}, \dot{y}, \dot{z})$  in terms of  $u^{a'} = (\dot{r}, \dot{\theta}, \dot{\phi})$ , and vice versa. Do the results match what you obtain by taking the time derivatives of Eqs. (4.6)?
3. Let  $x^a = (x, y, z)$  be rectangular coordinates, and let  $x^{a'} = (x', y', z')$  be a different rectangular coordinate system. The  $z$  and  $z'$  axes are the same, while the angle from the  $x$  axis to the  $x'$  axis is  $\theta$ . Compute the transformations  $\Lambda_a^{a'}$  and  $\Lambda_{a'}^a$ . Use these transformations to express the velocity  $\dot{x}^a = (\dot{x}, \dot{y}, \dot{z})$  in terms of  $\dot{x}^{a'} = (\dot{x}', \dot{y}', \dot{z}')$ , and vice versa. Are the results what you expect?
4. Verify that the metric  $g_{ab}$  and its inverse  $g^{ab}$  satisfy relationship (4.12), using metrics (4.11) and (4.14).
5. Compute the connection coefficients  $\Gamma_{bc}^a$  for cylindrical coordinates.
6. Write  $T^a_{b;c}$  in terms of  $T^a_b$  and its ordinary derivatives, in cylindrical coordinates.
7. Verify Eq. (4.35) for diagonal metrics.
8. Derive Eq. (4.40) for  $V_{;a}^a$ .
9. If the spherical components of the momentum density are not conserved, what meaning does "conservation of momentum" have?
10. Show that the choice of (4.60) for the diffusion coefficient leads to the monotonic first order scheme of Eq. (2.37).
11. Show that the mid-point fluxes (4.134) and (4.135) reproduce the standard second and fourth order finite difference approximations when used in the formula

$$\frac{\partial F}{\partial x} = \frac{F_{i+1/2} - F_{i-1/2}}{\Delta x}.$$



## Chapter 5

# Nonreflecting Boundary Conditions

Numerical solutions to hyperbolic systems of differential equations, such as the fluid dynamics equations, are usually obtained over a finite region. The previous chapters have focused on techniques for obtaining the solution interior to the boundaries of the system. However, the time evolution of the system is governed not only by the state in the interior of the region, but also by the choice of boundary conditions.

Many types of boundary conditions are possible. Fluid flows past solid objects (such as airplanes) require "solid wall" boundary conditions at the fluid-object interface. The normal velocity component must be zero at such a boundary, while the tangential velocity may or may not be zero (it is zero if viscosity is important in the boundary layer). Solid wall boundary conditions are discussed elsewhere (e.g., Beam and Warming [15], and Shih [16]), and will not be covered here.

One common boundary type is the free boundary, which corresponds to no solid wall or other physical interface, and across which matter and information are free to pass. In this case the evolution of the system depends on waves which enter the system from outside the boundary. The outgoing waves are described by characteristic equations, while the incoming waves depend on information which is external to the model volume. It often happens that the external solution is not known, in which case one may choose a boundary condition which allows waves in the interior (including shock waves) to pass out of the interior without generating reflections. These *nonreflecting boundary conditions*, originally postulated by Hedstrom [17] for the one dimensional case in rectangular geometry, have been generalized to the multidimensional case in arbitrary coordinate systems by Thompson [18], and are discussed below.

### 5.1 Waves in One Dimension

Consider first the one dimensional case in orthogonal (but not necessarily rectangular) coordinates. We have a system of  $n$  equations describing the behavior of  $n$  dependent

variables. Let  $\tilde{\mathbf{U}}$  be the vector<sup>1</sup> of conservative variables, satisfying

$$\frac{\partial \tilde{\mathbf{U}}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \mathbf{C}' = 0, \quad (5.1)$$

where  $\mathbf{F}$  is the flux vector, and  $\mathbf{C}'$  is an inhomogeneous term not containing derivatives (which often arises from divergence terms in nonrectangular geometry). Eq. (5.1) describes the conservation properties of the system; that is, it relates the rate of change of the integral of a field over a small volume to the flux of that field across the volume boundaries.

An alternate form for Eq. (5.1) is the primitive system, with a vector of dependent variables  $\mathbf{U}$ , which satisfies

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{U}}{\partial x} + \mathbf{C} = 0, \quad (5.2)$$

where  $\mathbf{A}$  is an  $n \times n$  matrix. The choice of primitive variable vector  $\mathbf{U}$  is not unique (although the choice of conserved variables is), and could be defined as the conservative vector. The following analysis assumes that  $\mathbf{U}$  and  $\tilde{\mathbf{U}}$  are distinct.

The two systems are related by

$$\frac{\partial \tilde{\mathbf{U}}}{\partial t} = \mathbf{P} \frac{\partial \mathbf{U}}{\partial t}, \quad (5.3)$$

$$\frac{\partial \mathbf{F}}{\partial x} = \mathbf{Q} \frac{\partial \mathbf{U}}{\partial x}, \quad (5.4)$$

with

$$P_{ij} = \frac{\partial \tilde{U}_i}{\partial U_j}, \quad (5.5)$$

$$Q_{ij} = \frac{\partial F_i}{\partial U_j}, \quad (5.6)$$

and

$$\mathbf{A} = \mathbf{P}^{-1} \mathbf{Q}, \quad (5.7)$$

$$\mathbf{C} = \mathbf{P}^{-1} \mathbf{C}', \quad (5.8)$$

where  $\mathbf{P}$  and  $\mathbf{Q}$  are also  $n \times n$  matrices.

Now let  $\mathbf{l}_i$  and  $\mathbf{r}_i$  be the set of left (row) and right (column) eigenvectors of  $\mathbf{A}$ , satisfying

$$\mathbf{l}_i \mathbf{A} = \lambda_i \mathbf{l}_i, \quad (5.9)$$

$$\mathbf{A} \mathbf{r}_i = \lambda_i \mathbf{r}_i, \quad (5.10)$$

where the  $\lambda_i$  are  $n$  eigenvalues of  $\mathbf{A}$ , ordered so that  $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ . (The system is hyperbolic if the eigenvalues of  $\mathbf{A}$  are real.) Then we obtain a diagonal matrix  $\Lambda$  by the similarity transformation

$$\mathbf{S} \mathbf{A} \mathbf{S}^{-1} = \Lambda, \quad (5.11)$$

<sup>1</sup>In this chapter, the term "vector" refers to any set of variables, and is not a vector in the tensor sense described in Chapter 4.



where the rows of  $S$  are the left eigenvectors  $l_i$ , the columns of  $S^{-1}$  are the right eigenvectors  $r_i$ , and the matrix  $A$  is diagonal, with  $A_{ii} = \lambda_i$ . (Note that the transformation follows from the orthogonality of the normalized left and right eigenvectors:  $l_i r_j = \delta_{ij}$ .)

Multiplying Eq. (5.2) by  $S$  gives

$$S \frac{\partial U}{\partial t} + AS \frac{\partial U}{\partial x} + SC = 0, \quad (5.12)$$

or

$$l_i \frac{\partial U}{\partial t} + \lambda_i l_i \frac{\partial U}{\partial x} + l_i C = 0, \quad (5.13)$$

in component form. Eq. (5.12) is the characteristic equation corresponding to the original forms (5.1) and (5.2).

If we can define a new function  $V$  by

$$dV_i = l_i dU + l_i C dt, \quad (5.14)$$

then (5.13) becomes

$$\frac{\partial V_i}{\partial t} + \lambda_i \frac{\partial V_i}{\partial x} = 0, \quad (5.15)$$

which is a set of wave equations for waves with characteristic velocities  $\lambda_i$ , as in Chapter 1. Each wave amplitude  $V_i$  is constant along the curve  $C_i$  in the  $xt$  plane defined by  $dx/dt = \lambda_i$ .

However, the definition of (5.14) generally can be made only if  $A$  and  $C$  are constant everywhere, or if no more than two differentials appear on the right side of (5.14). Otherwise the coefficients in (5.14) must satisfy Pfaff's condition for the integrability of differential forms for the functions  $V_i$  to exist [1], a condition not met for the fluid equations. Nevertheless, the characteristic form of (5.13) holds true independent of (5.14).

## 5.2 Nonreflecting Boundary Conditions in One Dimension

In the one dimensional case we wish to solve Eq. (5.1) over the region  $a \leq x \leq b$ . The problem is an initial boundary value problem, because both initial data in the region  $a \leq x \leq b$  and time dependent boundary conditions at  $x = a, b$  are needed for the problem to be well posed. Difficulty arises in the boundary condition specification because Eq. (5.1) generally contains eigenvalues of both signs at the boundaries, implying that waves are propagating into and out of the domain. It is therefore more fruitful to work with the characteristic form at the boundaries, since we can then consider each wave separately.

The outgoing waves (those with  $\lambda_i \leq 0$  at  $x = a$ , and  $\lambda_i \geq 0$  at  $x = b$ ) depend only on information at and within the boundaries. Thus those equations in the form of (5.13) which represent outgoing waves can be solved as is, or in any equivalent form. Properly designed numerical approximations to (5.13) for outgoing waves, which depend on one-sided finite difference approximations involving only interior and boundary points, will therefore be stable.

The incoming waves (with  $\lambda_i > 0$  at  $x = a$ , and  $\lambda_i < 0$  at  $x = b$ ) are another matter. They depend on data exterior to the boundary, and numerical approximations to (5.13) not involving exterior data will be unstable. Thus we need to know something about the exterior solution in order to specify useful boundary conditions. In some problems, particularly steady state aerodynamics problems, the far field solutions are known to a good approximation, and the appropriate values can be specified [19], [20].

For time dependent problems (and many steady state problems as well) it is often desirable to use so-called nonreflecting or radiation boundary conditions, which have the property of minimizing reflections from outgoing waves. A number of authors have attempted to create boundary conditions which have this nonreflecting property. Bayliss and Turkel [21] formulated a perturbation approach in which the perturbations about the desired steady state were expressed in terms of waves. They then imposed boundary conditions which annihilated the outgoing waves (i.e., prevented the generation of incoming waves). Engquist and Majda [22], [23] developed nonlocal, nonreflecting boundary conditions for linear systems. From their nonlocal conditions they derived a sequence of partially absorbing local conditions. Hedstrom [17] developed a nonreflecting boundary condition for the one dimensional rectangular, nonlinear case. As the only nonlinear condition, Hedstrom's is by far the most useful for time dependent problems. It will be generalized to multidimensional problems and non-rectangular coordinate systems below.

Hedstrom's nonreflecting boundary condition [17] can be stated in the following way: *the amplitudes of the incoming waves are constant, in time, at the boundaries.* This is the same as saying that there are no incoming waves, as it is the change in amplitude which indicates a wave. Mathematically, this condition is

$$\left. \frac{\partial V_i}{\partial t} \right|_{x=a,b} = 0, \quad (5.16)$$

in terms of the wave amplitude  $V_i$  of (5.14), or

$$\left( l_i \frac{\partial U}{\partial t} + l_i C \right) \Big|_{x=a,b} = 0, \quad (5.17)$$

in general, for those waves whose characteristic velocities are directed inward at the boundary. Eqs. (5.17) for the incoming waves and (5.13) for the outgoing waves completely determine the solution at the boundaries.

Note that Eq. (5.17) will not give the desired behavior for any problem which should in fact contain incoming waves. In such a case one must be able to specify something about the incoming waves. Fortunately, Eq. (5.17) seems to be adequate for many problems of interest.

It is easy to write a general equation which automatically reduces to Eq. (5.17) or Eq. (5.13) for incoming and outgoing waves. The general form is

$$\left( l_i \frac{\partial U}{\partial t} + \mathcal{L}_i + l_i C \right) \Big|_{x=a,b} = 0, \quad (5.18)$$

where

$$\mathcal{L}_i = \begin{cases} \lambda_i l_i \frac{\partial U}{\partial x} & \text{for outgoing waves,} \\ 0 & \text{for incoming waves.} \end{cases} \quad (5.19)$$

Thus the characteristic and nonreflecting boundary conditions can be combined in a very natural way, unlike other extrapolation methods.

The set of equations (5.18) is solved by a method of lines approach, in a way similar to (and along with) that for the conservative equations in the interior (as described in section 6). The function values are obtained at the discrete coordinate positions  $x_i$ , where

$$x_i = a + i\Delta x, \quad (5.20)$$

$$\Delta x = (b - a)/I. \quad (5.21)$$

Eq. (5.1) is solved at the interior points, defined by  $0 \leq i \leq I$ , while the boundary equation (in the form of Eq. (5.25) below) is solved at the boundary points, defined by  $i < 0$  or  $i > I$ . (An interior scheme which uses fourth order finite difference operators requires two boundary points at each boundary.) The spatial derivatives in (5.19) are evaluated using one sided difference approximations

$$\left. \frac{\partial U}{\partial x} \right|_i = \frac{1}{\Delta x} (U_{i+1} - U_i) \quad i < 0, \quad (5.22)$$

$$= \frac{1}{\Delta x} (U_i - U_{i-1}) \quad i > I. \quad (5.23)$$

To get an equation for the conservative variables, we first define  $\mathcal{L}$  as the column vector whose components are  $\mathcal{L}_i$ , and write

$$S \frac{\partial U}{\partial t} + \mathcal{L} + SC = 0, \quad (5.24)$$

which leads to

$$\frac{\partial \tilde{U}}{\partial t} + P(S^{-1}\mathcal{L} + C) = 0. \quad (5.25)$$

### 5.3 Waves in Two Dimensions

In two dimensions the conservative system is

$$\frac{\partial \tilde{U}}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + C'_x + C'_y = 0, \quad (5.26)$$

with  $C'_x$  and  $C'_y$  representing non-derivative terms, as before. (Only the sum of the  $C'$  terms matters; the sum has been partitioned into two terms to retain consistency with the one dimensional case.) We have the relations

$$\frac{\partial \tilde{U}}{\partial t} = P \frac{\partial U}{\partial t}, \quad (5.27)$$

$$\frac{\partial F}{\partial x} = Q \frac{\partial U}{\partial x}, \quad \frac{\partial G}{\partial y} = R \frac{\partial U}{\partial y}, \quad (5.28)$$

$$A = P^{-1}Q, \quad B = P^{-1}R, \quad (5.29)$$

$$C_x = P^{-1}C'_x, \quad C_y = P^{-1}C'_y, \quad (5.30)$$

which relate the conservative form of (5.26) to the following primitive form:

$$\frac{\partial U}{\partial t} + A \frac{\partial U}{\partial x} + B \frac{\partial U}{\partial y} + C_x + C_y = 0. \quad (5.31)$$

Now let  $l_i$ ,  $r_i$ , and  $\lambda_i$  be the left and right eigenvectors and eigenvalues of  $A$ . Similarly, let  $m_i$ ,  $s_i$ , and  $\mu_i$  be the left and right eigenvectors and eigenvalues of  $B$ . Then the matrices  $A$  and  $B$  can be put in the diagonal forms  $\Lambda$  and  $M$  by the similarity transformations

$$SAS^{-1} = \Lambda, \quad TBT^{-1} = M. \quad (5.32)$$

The rows of  $S$  ( $T$ ) are the left eigenvectors  $l_i$  ( $m_i$ ), the columns of  $S^{-1}$  ( $T^{-1}$ ) are the right eigenvectors  $r_i$  ( $s_i$ ), and  $\Lambda$  ( $M$ ) is the diagonal matrix of eigenvalues  $\lambda_i$  ( $\mu_i$ ). Then Eq. (5.31) can be rewritten as

$$\frac{\partial U}{\partial t} + S^{-1}\Lambda S \frac{\partial U}{\partial x} + T^{-1}MT \frac{\partial U}{\partial y} + C_x + C_y = 0. \quad (5.33)$$

which is as close to the characteristic form in one dimension as we can come unless  $S$  and  $T$  are the same (i.e., unless  $A$  and  $B$  are simultaneously diagonalizable), and which will be referred to as a characteristic form due to the presence of the diagonal characteristic velocity matrices.

## 5.4 Nonreflecting Boundary Conditions in Two Dimensions

The two dimensional problem allows for an arbitrary number of boundary points, since the boundary is now a curve enclosing a two dimensional space. Let the spatial coordinates be  $(x, y)$ , in a general curvilinear coordinate system (not necessarily rectangular). The solution  $U_{ij}$  is obtained at the points  $(x_i, y_j)$  on a rectangular grid with equal spacings  $(\Delta x, \Delta y)$  between successive points in each direction. Interior points have  $0 \leq i \leq I$ ,  $0 \leq j \leq J$ . The boundaries form a rectangle in the  $xy$  plane, and each side of the rectangle consists of one or more layers of boundary points. The boundary surfaces intersect at four corners, each of which consists of one or more corner points. Away from the corners, each boundary point has an associated normal and tangential direction (there would be two tangential directions in three dimensions), while at the corner points each direction is normal.

The original conservative system of equations is given in (5.26). For definiteness, let us consider the  $y$  boundaries, defined by the surfaces  $y=\text{constant}$ , which have the index values  $j < 0$  or  $j > J$ . Then the  $x$  derivative, which is in the tangential direction, can be

evaluated numerically as an interior term. The  $y$  term is in the normal direction, however, and must be put in characteristic form so that the appropriate boundary conditions can be imposed. Thus we write Eq. (5.26) as

$$\frac{\partial \tilde{U}}{\partial t} + \frac{\partial F}{\partial x} + C'_x + P \left( T^{-1} M T \frac{\partial U}{\partial y} + C_y \right) = 0 \quad (5.34)$$

at the  $y$  boundaries. Abbreviating the quantity in parentheses as  $-\partial U / \partial t_y$ , we must evaluate  $\partial U / \partial t_y$ , as given by

$$T \frac{\partial U}{\partial t_y} + M T \frac{\partial U}{\partial y} + T C_y = 0, \quad (5.35)$$

to provide boundary conditions for (5.34) at  $y$  boundaries. Next define the quantity  $M_k$ :

$$M_k = \begin{cases} \mu_k m_k \frac{\partial U}{\partial y} & \text{for outgoing waves,} \\ 0 & \text{for incoming waves,} \end{cases} \quad (5.36)$$

and compute  $\partial U / \partial t_y$  from

$$m_k \frac{\partial U}{\partial t_y} + M_k + m_k C_y = 0. \quad (5.37)$$

The spatial derivative in (5.36) is approximated by the one sided difference formulas

$$\left. \frac{\partial U}{\partial y} \right|_{ij} = \frac{1}{\Delta y} (U_{ij+1} - U_{ij}) \quad j < 0, \quad (5.38)$$

$$= \frac{1}{\Delta y} (U_{ij} - U_{ij-1}) \quad j > J. \quad (5.39)$$

Given  $\partial U / \partial t_y$ , we compute  $\partial \tilde{U} / \partial t$  from

$$\frac{\partial \tilde{U}}{\partial t} + \frac{\partial F}{\partial x} + C'_x = P \frac{\partial U}{\partial t_y} \quad (5.40)$$

At the  $x$  boundaries the  $y$  derivatives are evaluated in conservative form by centered difference approximations, while the  $x$  direction terms are put in characteristic form as above. At the corners both directions are normal, and all terms are put in characteristic form, as in (5.33).

## 5.5 Numerical Solution of the Interior Problem

The problems considered in this chapter are of two types. The first is the one dimensional fluid dynamics problem, in either rectangular or spherical coordinates. The second is a two dimensional problem in rectangular coordinates. In both cases the solutions may

be discontinuous, and it is necessary to add dissipative terms to the finite difference approximations in order to damp nonphysical oscillations around the discontinuities, as discussed in Chapters 2 and 4.

The one dimensional system, in conservative form and with dissipative terms included, may be written

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^n} \frac{\partial}{\partial r} (r^n \rho v) = \frac{1}{r^n} \frac{\partial}{\partial r} \left( r^n \kappa \frac{\partial \rho}{\partial r} \right), \quad (5.41)$$

$$\frac{\partial m}{\partial t} + \frac{1}{r^n} \frac{\partial}{\partial r} (r^n m v) + \frac{\partial p}{\partial r} = \frac{1}{r^n} \frac{\partial}{\partial r} \left( r^n \kappa \frac{\partial m}{\partial r} \right) - n \frac{\kappa}{r^2} m, \quad (5.42)$$

$$\frac{\partial e}{\partial t} + \frac{1}{r^n} \frac{\partial}{\partial r} [r^n (e + p) v] = \frac{1}{r^n} \frac{\partial}{\partial r} \left( r^n \kappa \frac{\partial e}{\partial r} \right), \quad (5.43)$$

where  $\rho$  is the density,  $v$  the velocity,  $m$  the momentum density ( $m = \rho v$ ),  $e$  the energy density ( $e = \frac{1}{2} \rho v^2 + p/(\gamma - 1)$ ), and  $p$  the pressure of the fluid. The equation of state can be written

$$p = (\gamma - 1) \left( e - \frac{1}{2} \rho v^2 \right), \quad (5.44)$$

where  $\gamma$  is the constant ratio of specific heats. The spatial coordinate is  $r$ , and the coordinate system is specified by  $n$  ( $n = 0, 1$ , or  $2$  for rectangular, cylindrical, or spherical coordinates, respectively). The dissipation coefficient  $\kappa$  and finite difference methods are given in Chapters 2 and 4. Fourth order finite difference approximations are made to the spatial derivatives in the convective and pressure gradient terms. The resulting semi-discrete equations are integrated in time according to the method of (2.31). The boundary equations (5.25) are integrated along with the interior equations, using the same time stepping scheme.

The two dimensional system, also in conservative form and containing dissipative terms, but in rectangular coordinates, is

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v_x) + \frac{\partial}{\partial y} (\rho v_y) = \frac{\partial}{\partial x} \left( \kappa \frac{\partial \rho}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial \rho}{\partial y} \right), \quad (5.45)$$

$$\frac{\partial m_x}{\partial t} + \frac{\partial}{\partial x} (m_x v_x) + \frac{\partial}{\partial y} (m_x v_y) + \frac{\partial p}{\partial x} = \frac{\partial}{\partial x} \left( \kappa \frac{\partial m_x}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial m_x}{\partial y} \right), \quad (5.46)$$

$$\frac{\partial m_y}{\partial t} + \frac{\partial}{\partial x} (m_y v_x) + \frac{\partial}{\partial y} (m_y v_y) + \frac{\partial p}{\partial y} = \frac{\partial}{\partial x} \left( \kappa \frac{\partial m_y}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial m_y}{\partial y} \right), \quad (5.47)$$

$$\frac{\partial e}{\partial t} + \frac{\partial}{\partial x} [(e + p) v_x] + \frac{\partial}{\partial y} [(e + p) v_y] = \frac{\partial}{\partial x} \left( \kappa \frac{\partial e}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial e}{\partial y} \right), \quad (5.48)$$

where  $(m_x, m_y)$  and  $(v_x, v_y)$  are the momentum density and velocity vectors, respectively. The equation of state is

$$p = (\gamma - 1) \left[ e - \frac{1}{2} \rho (v_x^2 + v_y^2) \right]. \quad (5.49)$$

## 5.6 Characteristic Equations for Fluid Dynamics

The boundary conditions require that the fluid equations be put in characteristic form at the boundaries, so we begin the boundary specification for fluid dynamics problems by finding the characteristic form for the fluid equations.

In the one dimensional case we can write the fluid equations in the form of Eq. (5.2) with

$$\mathbf{U} = \begin{pmatrix} \rho \\ v \\ s \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} v & \rho & 0 \\ \frac{c^2}{\rho} & v & \frac{p}{\rho s} \\ 0 & 0 & v \end{pmatrix}, \quad \mathbf{C} = \begin{pmatrix} \frac{n}{r} \rho v \\ 0 \\ 0 \end{pmatrix}, \quad (5.50)$$

where  $s$  is a measure of the entropy

$$s = p\rho^{-\gamma}, \quad (5.51)$$

and  $c$  is the speed of sound

$$c^2 = \gamma p / \rho. \quad (5.52)$$

(The dissipative terms are set to zero at the boundaries.)

The eigenvalues of  $\mathbf{A}$  are

$$\lambda_1 = v - c, \quad \lambda_2 = v, \quad \lambda_3 = v + c, \quad (5.53)$$

and the left eigenvectors are

$$\mathbf{l}_1 = \left(-c, \rho, -\frac{p}{sc}\right), \quad \mathbf{l}_2 = (0, 0, 1), \quad \mathbf{l}_3 = \left(c, \rho, \frac{p}{sc}\right). \quad (5.54)$$

Taking  $s$  as a primitive variable simplifies the eigenvalue calculation, but is inconvenient for numerical work. Therefore we eliminate  $s$  in favor of  $\rho$  and  $p$  and get the characteristic equations

$$\frac{\partial p}{\partial t} - \rho c \frac{\partial v}{\partial t} + \lambda_1 \left( \frac{\partial p}{\partial r} - \rho c \frac{\partial v}{\partial r} \right) + \frac{n}{r} \rho c^2 v = 0, \quad (5.55)$$

$$\frac{\partial p}{\partial t} - c^2 \frac{\partial \rho}{\partial t} + \lambda_2 \left( \frac{\partial p}{\partial r} - c^2 \frac{\partial \rho}{\partial r} \right) = 0, \quad (5.56)$$

$$\frac{\partial p}{\partial t} + \rho c \frac{\partial v}{\partial t} + \lambda_3 \left( \frac{\partial p}{\partial r} + \rho c \frac{\partial v}{\partial r} \right) + \frac{n}{r} \rho c^2 v = 0, \quad (5.57)$$

where the new primitive variable vector  $\mathbf{U}$  has components  $\rho$ ,  $v$ , and  $p$ .

Given  $\partial \mathbf{U} / \partial t$  at the boundaries,  $\partial \tilde{\mathbf{U}} / \partial t$  is obtained from (5.3) by

$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial t}, \quad (5.58)$$

$$\frac{\partial m}{\partial t} = v \frac{\partial \rho}{\partial t} + \rho \frac{\partial v}{\partial t}, \quad (5.59)$$

$$\frac{\partial e}{\partial t} = \frac{1}{2} v^2 \frac{\partial \rho}{\partial t} + \rho v \frac{\partial v}{\partial t} + \frac{1}{\gamma - 1} \frac{\partial p}{\partial t}. \quad (5.60)$$

In two dimensions the fluid equations may be written in the form of (5.33) with

$$\mathbf{U} = \begin{pmatrix} \rho \\ v_x \\ v_y \\ s \end{pmatrix}, \mathbf{A} = \begin{pmatrix} v_x & \rho & 0 & 0 \\ \frac{c^2}{\rho} & v_x & 0 & \frac{p}{\rho s} \\ 0 & 0 & v_x & 0 \\ 0 & 0 & 0 & v_x \end{pmatrix}, \mathbf{B} = \begin{pmatrix} v_y & 0 & \rho & 0 \\ 0 & v_y & 0 & 0 \\ \frac{c^2}{\rho} & 0 & v_y & \frac{p}{\rho s} \\ 0 & 0 & 0 & v_y \end{pmatrix}, C_x = C_y = 0. \quad (5.61)$$

The eigenvalues of  $\mathbf{A}$  and  $\mathbf{B}$  are

$$\lambda_1 = v_x - c, \quad \lambda_2 = \lambda_3 = v_x, \quad \lambda_4 = v_x + c, \quad (5.62)$$

$$\mu_1 = v_y - c, \quad \mu_2 = \mu_3 = v_y, \quad \mu_4 = v_y + c. \quad (5.63)$$

The  $y$  direction characteristic terms, in the form of (5.35), are

$$\frac{\partial p}{\partial t_y} - \rho c \frac{\partial v_y}{\partial t_y} + \mu_1 \left( \frac{\partial p}{\partial y} - \rho c \frac{\partial v_y}{\partial y} \right) = 0, \quad (5.64)$$

$$\frac{\partial v_x}{\partial t_y} + \mu_2 \frac{\partial v_x}{\partial y} = 0, \quad (5.65)$$

$$\frac{\partial p}{\partial t_y} - c^2 \frac{\partial \rho}{\partial t_y} + \mu_3 \left( \frac{\partial p}{\partial y} - c^2 \frac{\partial \rho}{\partial y} \right) = 0, \quad (5.66)$$

$$\frac{\partial p}{\partial t_y} + \rho c \frac{\partial v_y}{\partial t_y} + \mu_4 \left( \frac{\partial p}{\partial y} + \rho c \frac{\partial v_y}{\partial y} \right) = 0. \quad (5.67)$$

An analogous set holds for the  $x$  direction.

The conservative and primitive time derivatives are related by

$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial t}, \quad (5.68)$$

$$\frac{\partial m_x}{\partial t} = v_x \frac{\partial \rho}{\partial t} + \rho \frac{\partial v_x}{\partial t}, \quad (5.69)$$

$$\frac{\partial m_y}{\partial t} = v_y \frac{\partial \rho}{\partial t} + \rho \frac{\partial v_y}{\partial t}, \quad (5.70)$$

$$\frac{\partial e}{\partial t} = \frac{1}{2} (v_x^2 + v_y^2) \frac{\partial \rho}{\partial t} + \rho \left( v_x \frac{\partial v_x}{\partial t} + v_y \frac{\partial v_y}{\partial t} \right) + \frac{1}{\gamma - 1} \frac{\partial p}{\partial t}. \quad (5.71)$$



## 5.7 Boundary Conditions for Fluid Dynamics

In the one dimensional case, we solve Eqs. (5.41)–(5.43) in the interior using centered finite difference approximations for the spatial derivatives, and an explicit ordinary differential equation solver to integrate the time derivatives of the conservative variables. The interior algorithm requires data at the boundary points, which are obtained by solving the combined characteristic and nonreflecting equations at those points. The details of the boundary calculations are given below.

We first write the boundary equations as

$$\frac{dp_i}{dt} - \rho_i c_i \frac{dv_i}{dt} + \mathcal{L}_{1i} + \frac{n}{r_i} \rho_i c_i^2 v_i = 0, \quad (5.72)$$

$$\frac{dp_i}{dt} - c_i^2 \frac{d\rho_i}{dt} + \mathcal{L}_{2i} = 0, \quad (5.73)$$

$$\frac{dp_i}{dt} + \rho_i c_i \frac{dv_i}{dt} + \mathcal{L}_{3i} + \frac{n}{r_i} \rho_i c_i^2 v_i = 0, \quad (5.74)$$

where each  $\mathcal{L}_{ki}$  is set to zero if  $\lambda_k$  at  $r_i$  is directed inward (nonreflecting condition), or is computed according to the characteristic equations if  $\lambda_k$  at  $r_i$  is directed outward:

$$\mathcal{L}_{1i} = (v_i - c_i) \frac{1}{\Delta r} [p_{i+1} - p_i - \rho_i c_i (v_{i+1} - v_i)] \quad i < 0, \quad v_i - c_i < 0, \quad (5.75)$$

$$= (v_i - c_i) \frac{1}{\Delta r} [p_i - p_{i-1} - \rho_i c_i (v_i - v_{i-1})] \quad i > I, \quad v_i - c_i > 0; \quad (5.76)$$

$$\mathcal{L}_{2i} = v_i \frac{1}{\Delta r} [p_{i+1} - p_i - c_i^2 (\rho_{i+1} - \rho_i)] \quad i < 0, \quad v_i < 0, \quad (5.77)$$

$$= v_i \frac{1}{\Delta r} [p_i - p_{i-1} - c_i^2 (\rho_i - \rho_{i-1})] \quad i > I, \quad v_i > 0; \quad (5.78)$$

$$\mathcal{L}_{3i} = (v_i + c_i) \frac{1}{\Delta r} [p_{i+1} - p_i + \rho_i c_i (v_{i+1} - v_i)] \quad i < 0, \quad v_i + c_i < 0, \quad (5.79)$$

$$= (v_i + c_i) \frac{1}{\Delta r} [p_i - p_{i-1} + \rho_i c_i (v_i - v_{i-1})] \quad i > I, \quad v_i + c_i > 0. \quad (5.80)$$

Given the  $\mathcal{L}$  values, the time derivatives of the primitive variables are

$$\frac{dp_i}{dt} = -\frac{1}{2}(\mathcal{L}_{3i} + \mathcal{L}_{1i}) - \frac{n}{r_i} \rho_i c_i^2 v_i, \quad (5.81)$$

$$\frac{dv_i}{dt} = -\frac{1}{2\rho_i c_i}(\mathcal{L}_{3i} - \mathcal{L}_{1i}), \quad (5.82)$$

$$\frac{d\rho_i}{dt} = \frac{1}{c_i^2} \left( \frac{dp_i}{dt} + \mathcal{L}_{2i} \right), \quad (5.83)$$

and Eqs. (5.59) and (5.60) provide  $dm_i/dt$  and  $de_i/dt$  at the boundaries, to be integrated in time along with the interior values.

The two dimensional case is similar. We solve Eqs. (5.45)–(5.48) in the interior, using centered finite difference approximations for the spatial derivative, and an explicit

integration method for the time derivatives. We now have four boundaries, defined by  $x = x_{min}$ ,  $x = x_{max}$ ,  $y = y_{min}$ , and  $y = y_{max}$ . Since all four boundaries are treated in a similar fashion, it will be sufficient to look at the  $y=\text{constant}$  boundaries.

We begin by writing the fluid equations at the  $y$  boundary points as

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v_x) - \frac{\partial \rho}{\partial t_y} = \frac{\partial}{\partial x} \left( \kappa \frac{\partial \rho}{\partial x} \right), \quad (5.84)$$

$$\frac{\partial m_x}{\partial t} + \frac{\partial}{\partial x}(m_x v_x) + \frac{\partial p}{\partial x} - \frac{\partial m_x}{\partial t_y} = \frac{\partial}{\partial x} \left( \kappa \frac{\partial m_x}{\partial x} \right), \quad (5.85)$$

$$\frac{\partial m_y}{\partial t} + \frac{\partial}{\partial x}(m_y v_x) - \frac{\partial m_y}{\partial t_y} = \frac{\partial}{\partial x} \left( \kappa \frac{\partial m_y}{\partial x} \right), \quad (5.86)$$

$$\frac{\partial e}{\partial t} + \frac{\partial}{\partial x}[(e + p)v_x] - \frac{\partial e}{\partial t_y} = \frac{\partial}{\partial x} \left( \kappa \frac{\partial e}{\partial x} \right), \quad (5.87)$$

where the  $\partial \tilde{U} / \partial t_y$  terms are the contributions to  $\partial \tilde{U} / \partial t$  due to derivatives in the normal ( $y$ ) direction. The  $x$  derivatives are in the tangential direction, relative to the boundary, and are evaluated just as in the interior.

We need to compute the  $\partial \tilde{U} / \partial t_y$  terms in Eqs. (5.84)–(5.87), and begin by writing Eqs. (5.64)–(5.67) in finite difference form, as

$$\frac{dp_{ij}}{dt_y} - \rho_{ij} c_{ij} \frac{dv_{yij}}{dt_y} + M_{1ij} = 0, \quad (5.88)$$

$$\frac{dv_{xij}}{dt_y} + M_{2ij} = 0, \quad (5.89)$$

$$\frac{dp_{ij}}{dt_y} - c_{ij}^2 \frac{d\rho_{ij}}{dt_y} + M_{3ij} = 0, \quad (5.90)$$

$$\frac{dp_{ij}}{dt_y} + \rho_{ij} c_{ij} \frac{dv_{yij}}{dt_y} + M_{4ij} = 0, \quad (5.91)$$

where each  $M_{kij}$  is set to zero if the local  $y$  direction characteristic velocity,  $\mu_k$ , is directed inward (nonreflecting condition), or is computed according to the characteristic forms below if  $\mu_k$  is directed outward:

$$M_{1ij} = (v_{yij} - c_{ij}) \frac{1}{\Delta y} [p_{ij+1} - p_{ij} - \rho_{ij} c_{ij} (v_{yij+1} - v_{yij})] \quad j < 0, \quad v_{yij} - c_{ij} < 0, \quad (5.92)$$

$$= (v_{yij} - c_{ij}) \frac{1}{\Delta y} [p_{ij} - p_{ij-1} - \rho_{ij} c_{ij} (v_{yij} - v_{yij-1})] \quad j > J, \quad v_{yij} - c_{ij} > 0; \quad (5.93)$$

$$M_{2ij} = v_{yij} \frac{1}{\Delta y} (v_{xij+1} - v_{xij}) \quad j < 0, \quad v_{yij} < 0, \quad (5.94)$$

$$= v_{yij} \frac{1}{\Delta y} (v_{xij} - v_{xij-1}) \quad j > J, \quad v_{yij} > 0; \quad (5.95)$$

$$M_{3ij} = v_{yij} \frac{1}{\Delta y} [p_{ij+1} - p_{ij} - c_{ij}^2 (\rho_{ij+1} - \rho_{ij})] \quad j < 0, \quad v_{yij} < 0, \quad (5.96)$$

$$= v_{vij} \frac{1}{\Delta y} [p_{ij} - p_{ij-1} - c_{ij}^2 (\rho_{ij} - \rho_{ij-1})] \quad j > J, v_{vij} > 0; \quad (5.97)$$

$$M_{4ij} = (v_{vij} + c_{ij}) \frac{1}{\Delta y} [p_{ij+1} - p_{ij} + \rho_{ij} c_{ij} (v_{vij+1} - v_{vij})] \quad j < 0, v_{vij} + c_{ij} < 0, \quad (5.98)$$

$$= (v_{vij} + c_{ij}) \frac{1}{\Delta y} [p_{ij} - p_{ij-1} + \rho_{ij} c_{ij} (v_{vij} - v_{vij-1})] \quad j > J, v_{vij} + c_{ij} > 0. \quad (5.99)$$

Given the  $M$  values, we compute  $\partial U / \partial t_v$  from

$$\frac{dp_{ij}}{dt_v} = -\frac{1}{2} (M_{4ij} + M_{1ij}), \quad (5.100)$$

$$\frac{dv_{vij}}{dt_v} = -\frac{1}{2\rho_{ij}c_{ij}} (M_{4ij} - M_{1ij}), \quad (5.101)$$

$$\frac{dv_{zij}}{dt_v} = -M_{2ij}, \quad (5.102)$$

$$\frac{d\rho_{ij}}{dt_v} = \frac{1}{c_{ij}^2} \left( \frac{dp_{ij}}{dt_v} + M_{3ij} \right). \quad (5.103)$$

Finally,  $dm_{zij}/dt_v$ ,  $dm_{vij}/dt_v$ , and  $dc_{ij}/dt_v$  are calculated using (5.69)–(5.71), and their values are used in the finite difference approximations to Eqs. (5.84)–(5.87). A similar process is followed at the  $x$  boundaries.

## 5.8 Test Problems

It is instructive to see how well the combined interior and boundary methods described up to this point work in practice. To do so, we consider some test problems, in one and two dimensions.

As in Chapter 4, the one dimensional test problems are evaluated on a grid of unit length, divided into 100 subintervals ( $I = 100$ ,  $\Delta r = 0.01$ ). The value of  $\gamma$  in the equation of state is 5/3 throughout. The figures show the analytical solutions (solid lines) and numerical solutions (dots) for the density  $\rho$ , the pressure  $p$ , the momentum density  $m$ , and the velocity  $v$ , at a time  $t$ . The Courant number  $\sigma$ ,

$$\begin{aligned} \sigma &= \frac{c_r \Delta t}{\Delta r} & (1 \text{ dimension}), \\ &= \left( \frac{c_x}{\Delta x} + \frac{c_y}{\Delta y} \right) \Delta t & (2 \text{ dimensions}), \end{aligned} \quad (5.104)$$

is set to 1 throughout, where  $c_x = \max(|v_x| + c)$  over the grid (and similarly for  $c_y$  and  $c_r$ ).

The first problem is a single shock wave moving into a uniform stationary medium. The shock starts at  $x = 0.5$  and has a positive velocity. The pre-shock state has  $\rho = p = 1$  and  $v = 0$ . The problem is determined by the pre- and post-shock values of  $\rho$ ,  $p$ , and  $v$ , and the shock velocity  $V_s$ , and must satisfy the three shock jump conditions [12].

Thus we have one more free parameter, chosen to be the Mach number  $M = v/c$  of the post-shock flow. The Mach number is related to the ratio  $R = p_s/p_u$  of the shocked to unshocked pressures by

$$M^2 = \frac{2}{\gamma R} \frac{(R-1)^2}{\gamma + 1 + (\gamma-1)R}. \quad (5.105)$$

As  $R \rightarrow \infty$ ,  $M^2 \rightarrow M_{max}^2 = 2/[\gamma(\gamma-1)]$ , where  $M_{max} = 1.3416$  for  $\gamma = 5/3$ .

A reflection is generated when an outgoing subsonic shock wave crosses a boundary, as demonstrated by Hedstrom [17]. The reflection takes the form of a constant amplitude perturbation to the post-shock solution, which travels inward from the boundary at the speed of sound relative to the moving fluid. A convenient measure of the reflection is the relative error in the pressure after the shock has crossed the boundary, defined as the difference between the numerical and analytical pressure values, divided by the analytical pressure. Table 5.1 gives the pressure ratio  $R$  and reflections as a function of the Mach number, for subsonic shock waves modeled with the dissipation specified by  $k = 0.35$ . (A significantly smaller value of  $k$  results in large oscillations near the shock, while a larger value spreads the shock jump out over many grid points.)

The reflections are small, nowhere exceeding 1%. The worst case is the  $M = 0.98$  shock, with a reflection of 0.82%. It is interesting to note that the reflection decreases as  $M$  increases from 0.99 to 1.0, although the shock jump increases.

Hedstrom [17] observed a reflection of 12% in the velocity profile of his Figure 6. It is not certain why there is such a large discrepancy between his results and those presented here, but a likely culprit is the mismatch between his interior and boundary methods. He used the Lax-Wendroff method for the interior. At the boundary, he used first order approximations to the spatial derivatives, and

$$\left. \frac{\partial U}{\partial t} \right|_i^n = \frac{1}{\Delta t} (v_i^{n+1} - v_i^n) + O(\Delta t) \quad (5.106)$$

for the time derivatives. The two time integration methods are quite different. In contrast, the four step time integration scheme of (2.31) was used for both interior and boundary points here.

When the flow behind the shock is supersonic ( $M > 1$ ) all characteristics point to the right, and no signals can propagate to the left. Thus no reflections can be produced, and none are observed.

The next example is the shock tube problem, as described in section 4.9. At time  $t = 0$  the system consists of two spatially constant, stationary states, adjoining at  $x = 0$ . The left state ( $x < 0$ ) has  $\rho = p = 1$ , while the right state has  $\rho = 0.125$ ,  $p = 0.1$ .

Figure 5.1 shows the numerical solution at step 100 and  $t = 0.438$ , with  $k = 0.3$ . The rarefaction wave has passed through the left boundary, and the shock wave has passed through the right boundary. No reflections are visible on either side. The boundaries are well behaved.

The next problem considered is the Sedov solution for a spherically symmetric explosion, also described in section 4.9. Figure 5.2 shows the explosion at step 1000,  $t = 3.069$ , with  $k = 0.35$ , and with the vertical scales magnified relative to the example in Figure 4.8. The shock wave has passed out of the domain, and the velocity at the boundary has de-

Mach Number	Pressure Ratio	Relative Error (%)
$M$	$R = p_s/p_u$	$100 \times (p_{num} - p_{an})/p_{an}$
0.50	2.504	0.08
0.60	3.096	0.19
0.70	3.891	0.33
0.80	5.000	0.48
0.90	6.635	0.68
0.92	7.058	0.71
0.94	7.524	0.74
0.95	7.775	0.77
0.96	8.040	0.78
0.97	8.319	0.81
0.98	8.614	0.82
0.99	8.926	0.82
0.995	9.089	0.80
1.00	9.257	0.77

Table 5.1: Reflections for Subsonic Shocks

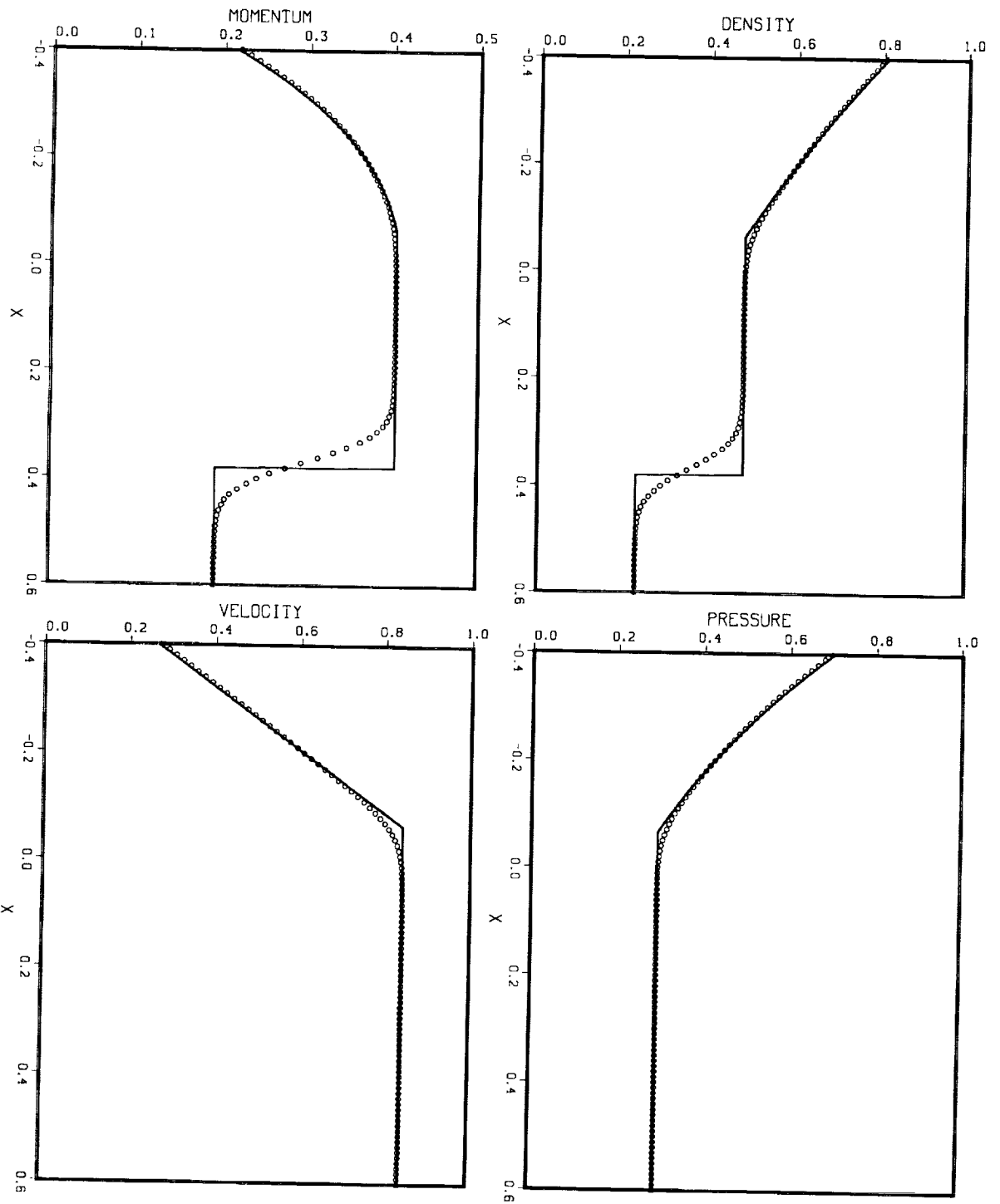


Figure 5.1: Shock tube at step 100

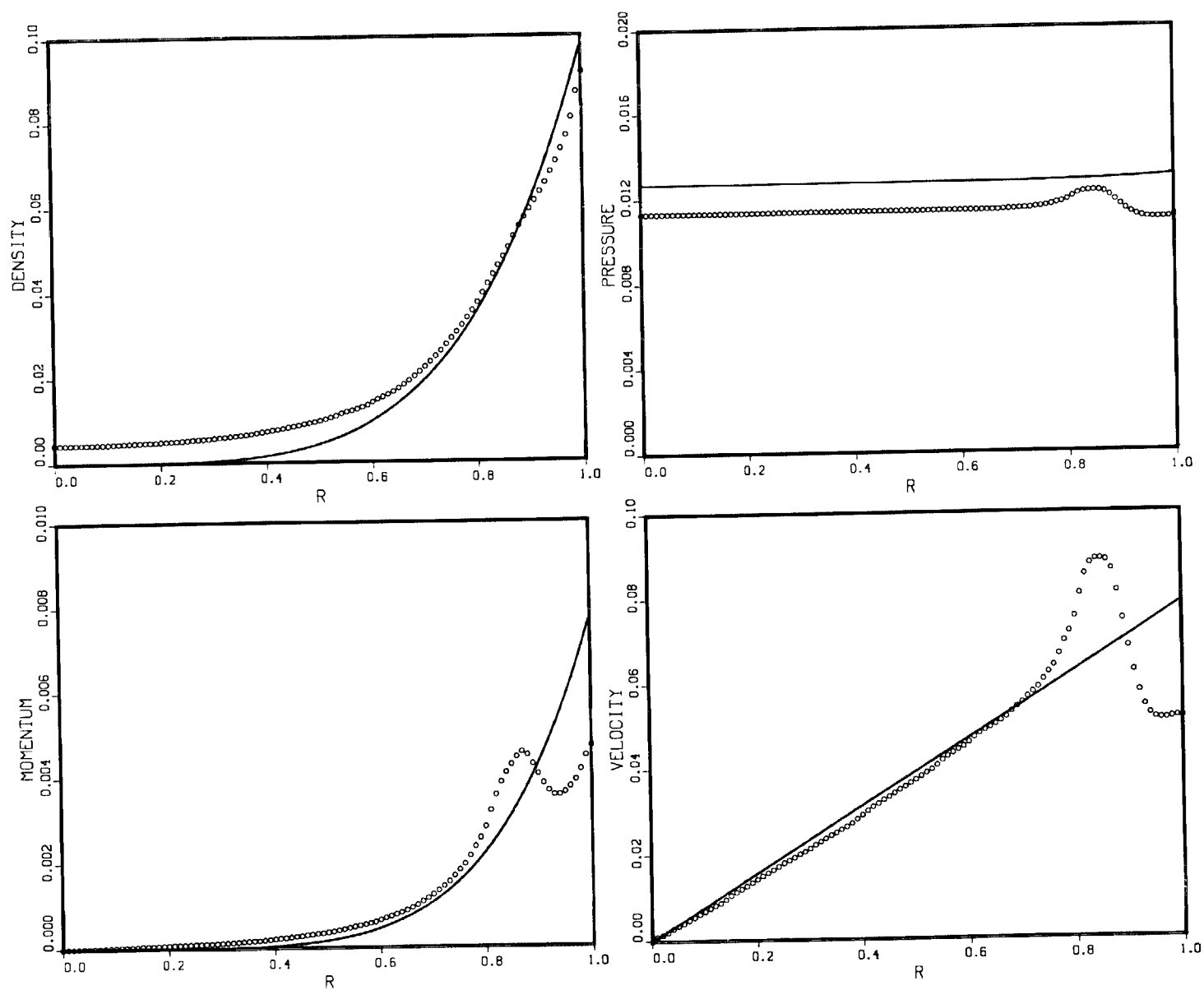


Figure 5.2: Spherical explosion at step 1000

creased from supersonic (immediately behind the shock) to subsonic. A perturbation has developed at the boundary and is propagating inward, as can be seen most clearly from the velocity curve. The discrepancy between the numerical and analytic solutions is presumably due to the fact that the similarity solution for the explosion really does contain an inward propagating wave, which is suppressed by the boundary conditions. The resulting numerical solution is a valid one, but it is not the solution to the explosion problem at late times.

The impossibility of properly specifying boundary conditions for all problems with the nonreflecting prescription is further illustrated by the following problem, the homologous expansion of a uniform medium. At time  $t = 0$  the density and pressure are uniform, with  $\rho = p = 1$ . The velocity is linear, with  $u = x/t_0$ ,  $t_0$  chosen to be 1. The region studied is  $-0.5 \leq x \leq 0.5$ . The density and pressure decrease with time but remain uniform, while the velocity also decreases but remains linear in  $x$ . The flow at the boundaries is always subsonic and directed outward for this set of initial conditions.

The problem has a simple analytical solution, given by

$$\rho = \rho_0 \left(1 + \frac{t}{t_0}\right)^{-1}, \quad (5.107)$$

$$p = p_0 \left(1 + \frac{t}{t_0}\right)^{-\gamma}, \quad (5.108)$$

$$v = \frac{x}{t + t_0}. \quad (5.109)$$

One can verify by direct substitution that this solution does not satisfy the nonreflecting boundary conditions. For example, at the right boundary ( $x = b$ ) the flow is subsonic and directed outward. The two characteristic equations representing outgoing waves (Eqs. (5.56) and (5.57)) hold as written, while the absence of an incoming wave is imposed by the nonreflecting condition of Eq. (5.72) with  $\mathcal{L}_1 = 0$ , which can be written

$$\frac{\partial p}{\partial t} - \rho c \frac{\partial v}{\partial t} = 0.$$

The analytic solution does not satisfy the nonreflecting condition, so the nonreflecting condition will not produce the desired numerical solution.

Figure 5.3 shows the expansion problem at step 50,  $t = 0.305$ , with  $k = 0$ . The numerical and analytical solutions diverge markedly near the boundaries, although they match well in the middle portion. The discrepancy grows with time until the two solutions disagree everywhere.

We can use information about this particular problem to specify better boundary conditions. In particular, the pressure gradient is zero everywhere, and the velocity satisfies

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} = 0, \quad (5.110)$$

which is in characteristic form and describes outflow at the boundary. If (5.110) is used in place of the nonreflecting boundary condition, we have three characteristic equations



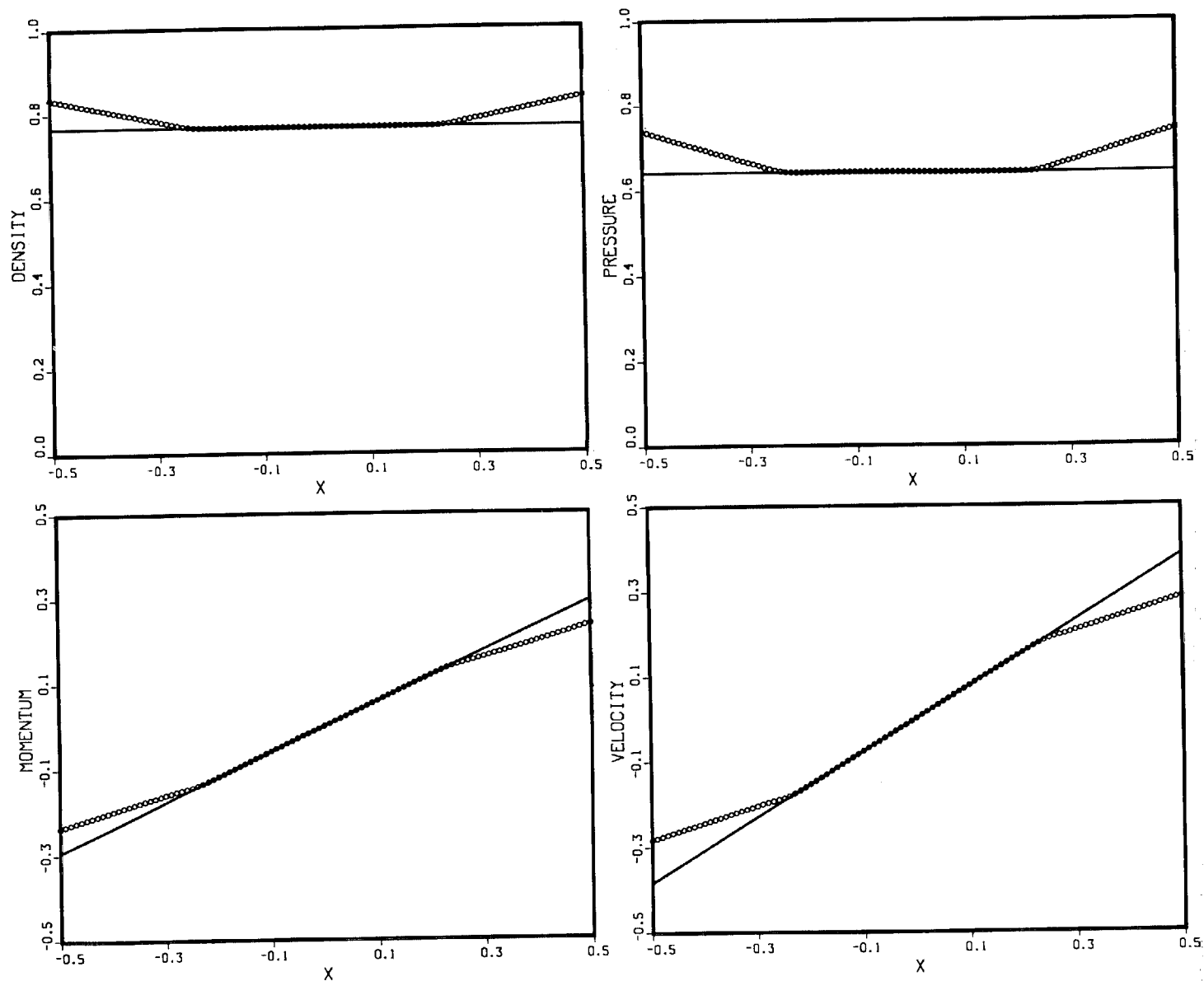


Figure 5.3: Homologous expansion at step 50

describing outgoing waves. (By throwing out the pressure gradient term, we have excluded sound waves from the problem. The only characteristic velocity left is the fluid velocity. The evolution of the velocity profile then determines the rest of the solution). The resulting numerical solution matches the analytical solution everywhere.

This result is not meant as an endorsement of Eq. (5.110) as a boundary condition in general (it does nothing useful for the explosion problem), but simply illustrates that nonreflecting boundary conditions cannot be expected to give the desired results on problems which do contain incoming waves. Information specific to such problems may be used to produce more useful boundary conditions.

The final test problem is two dimensional. It is a planar Newtonian shock, traveling in rectangular geometry. The grid has  $\Delta x = \Delta y = 1/130$ . The shock is traveling toward the upper right, at a  $45^\circ$  angle with respect to the  $x$  axis. The initial distance  $R_0$  between the shock front and the origin is 0.8. The unshocked density and pressure are  $\rho = 1$ ,  $p = 1$ , with  $v_x = v_y = 0$ . The Mach number of the flow behind the shock is  $M = 0.95$ , picked to roughly maximize reflection errors. The dissipation used is  $k = 0.3$ .

Contour plots of the density, pressure, and velocity fields in Figures 5.4, 5.5, and 5.6 show the time evolution of the solution. The arrows in the velocity plot show the direction of the flow, and have a length proportional to the magnitude of the velocity. The ratio of successive contour values is 1.01. The figures are at step 0,  $t = 0$ ; step 100,  $t = 0.098$ ; and step 200,  $t = 0.197$ , respectively. Step 0 shows the initial conditions. Step 100 shows the shock shortly before it reaches the corner. Small boundary perturbations can be seen near the edges of the shock. Step 200 shows the solution shortly after the shock has left the grid. The reflection from the corner has propagated inward, and at its peak amounts to about 6% of the post-shock pressure profile. The reflection is greater than in the one dimensional case, perhaps because the corner is subject to reflections from two coordinate directions, but not enough to obscure significant features of the post-shock flow (if there were any).

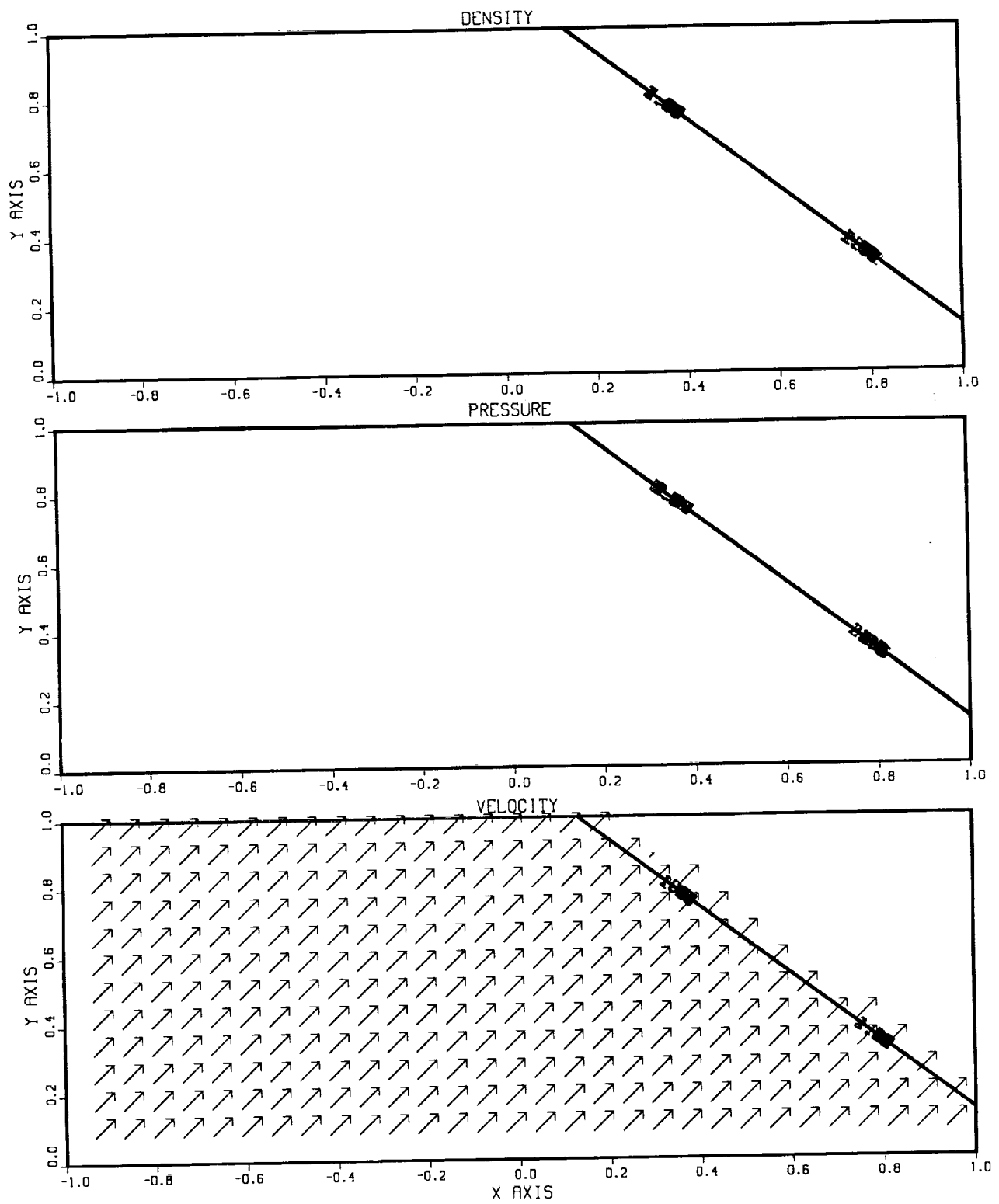


Figure 5.4: Angled shock at step 0

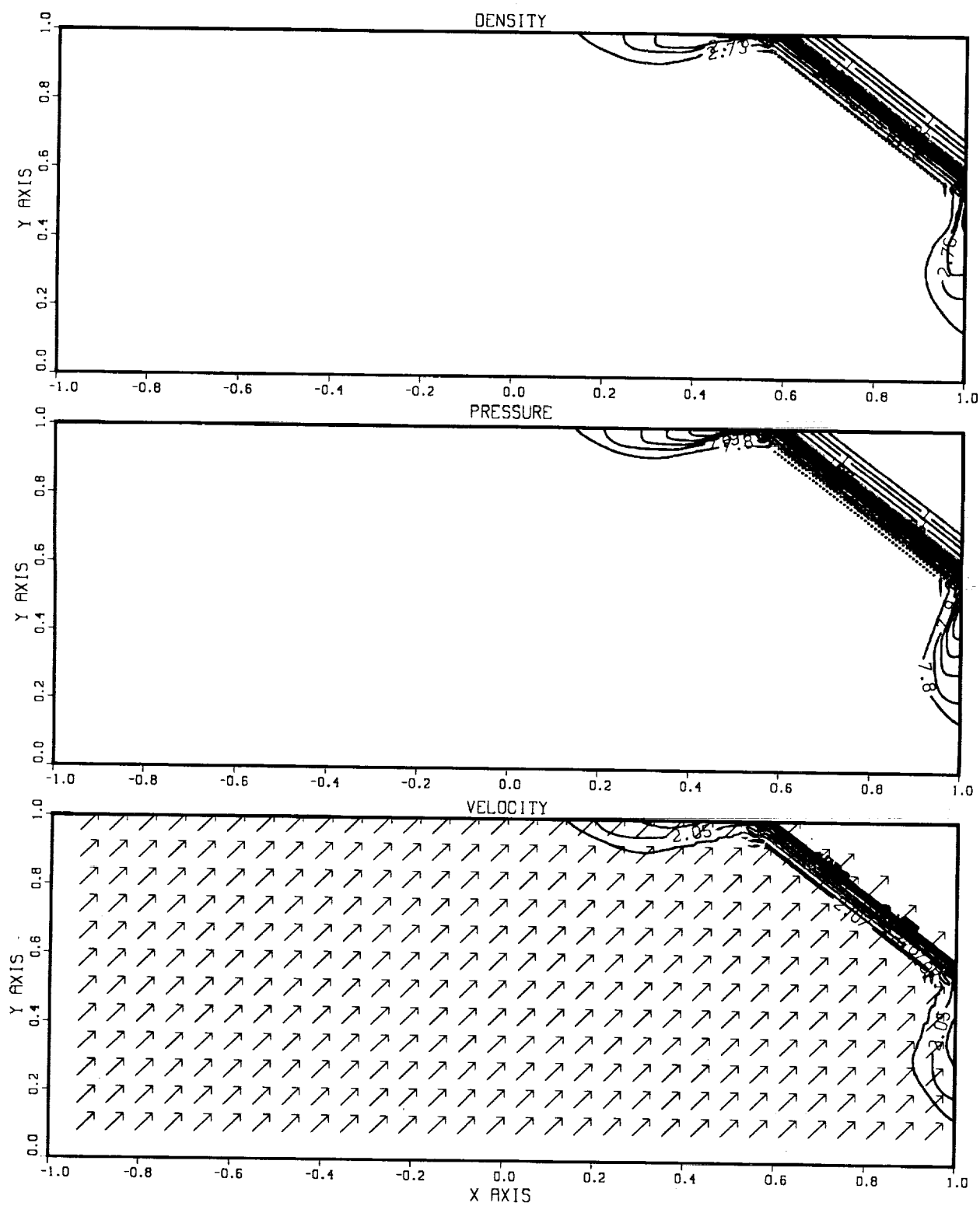


Figure 5.5: Angled shock at step 100

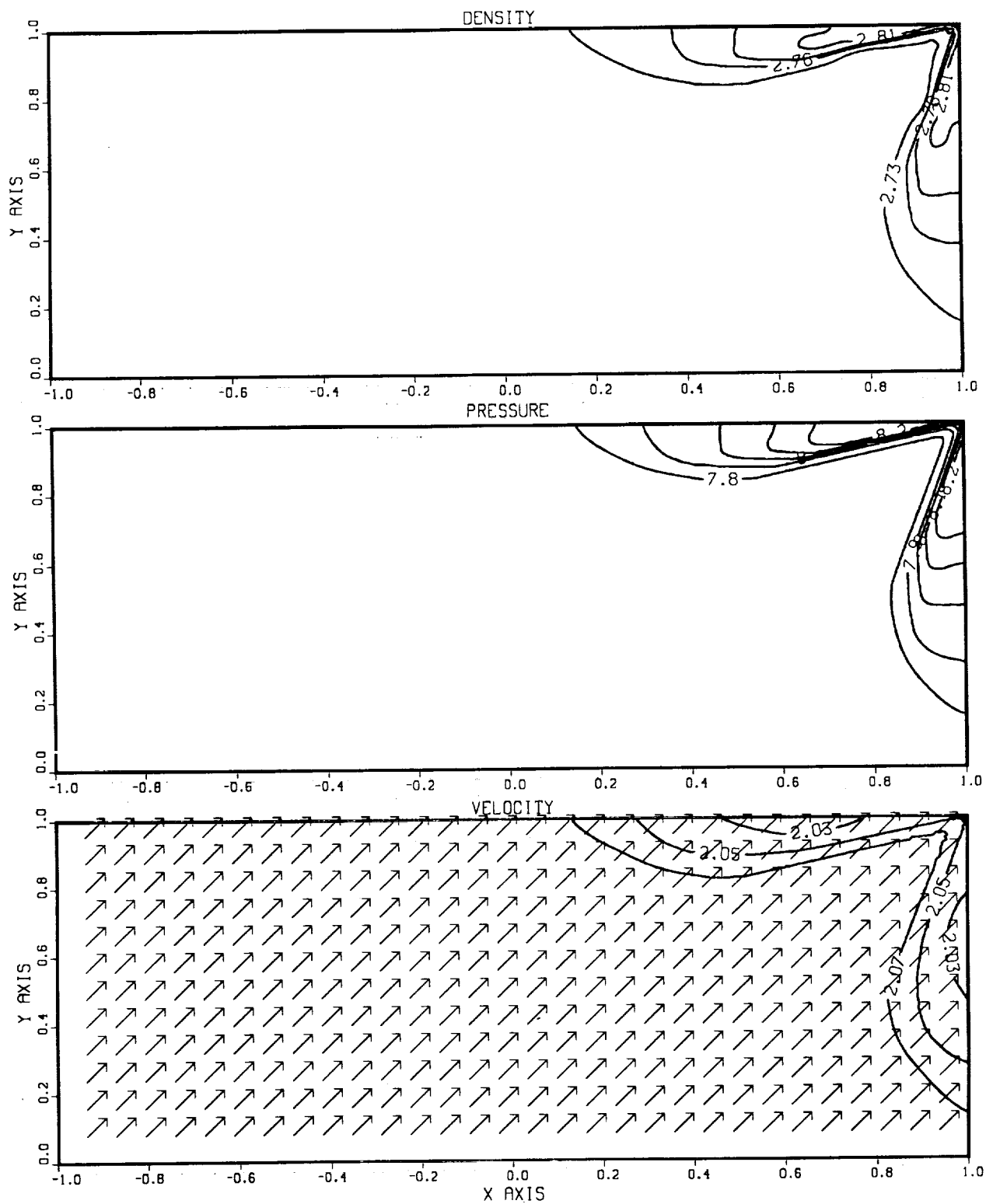


Figure 5.6: Angled shock at step 200

## 5.9 Exercises

1. Derive the primitive form of the fluid equations given in Eqs. (5.50) from the conservative form, in one dimension and in rectangular coordinates.
2. Starting with Eqs. (5.50), assume isentropic flow ( $s \equiv \text{constant}$ ), and show that only two characteristic equations result. What are the characteristic velocities?
3. Express the results of problem 2 in the form of Eq. (5.15). The two wave amplitudes  $V_1$  and  $V_2$  are called *Riemann invariants* in fluid dynamics. Each Riemann invariant is constant along its corresponding trajectory ( $v - c$  or  $v + c$ ) in the  $xt$  plane. Riemann invariants do not exist if the flow is non-isentropic.
4. Find the *right* eigenvectors of matrix  $A$  in Eq. (5.49). Form the similarity transformation matrices  $S$  and  $S^{-1}$ , and verify the similarity transformation of Eq. (5.11).
5. Derive the characteristic velocity components for the two dimensional fluid problem of Eq. (5.61).
6. Perform the shock wave calculation described in section 5.8, for a Mach number  $M = 0.9$ . Do you see a reflection? If so, how big is it?
7. Verify that the homologous expansion solution of Eq. (5.107)–(5.109) does not satisfy the nonreflecting boundary condition at the right boundary.

# Appendix A

## The Equations of Fluid Dynamics

Chapter 4 described the basic concepts of tensor calculus, the tensor formulation of the fluid dynamics equations, and artificial viscosity. This appendix provides a complete list of the relevant equations for fluid dynamics in rectangular, cylindrical, and spherical coordinate systems.

### A.1 Coordinate Geometries and Metric Tensors

The geometry of the coordinate system is described by the metric tensor  $g_{ab}$ . The metric tensor is a symmetric second rank tensor, whose components are usually functions of the coordinates. The metric tensor defines the physical distance  $ds$  between two closely space points, at  $x^a = (x^1, x^2, x^3)$  and  $x^a + dx^a = (x^1 + dx^1, x^2 + dx^2, x^3 + dx^3)$ , in terms of the coordinate differentials  $dx^a$ . This distance is given by

$$ds^2 = g_{ab} dx^a dx^b. \quad (\text{A.1})$$

The symmetry of the metric tensor implies that, in  $n$  dimensions, only  $n(n+1)/2$  of its  $n^2$  components may be unique (six components in three dimensions). A general metric in three dimensions may be written as a  $3 \times 3$  array of numbers,

$$g_{ab} = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix}, \quad (\text{A.2})$$

where by symmetry

$$g_{ab} = g_{ba}. \quad (\text{A.3})$$

In orthogonal coordinate systems, where the coordinate axes are perpendicular to

each other, the metric tensor is diagonal, and may be written

$$g_{ab} = \begin{pmatrix} h_1^2 & & \\ & h_2^2 & \\ & & h_3^2 \end{pmatrix}, \quad (\text{A.4})$$

where  $h_1$ ,  $h_2$ , and  $h_3$  are the scale factors for the coordinate directions (and the superscript 2 represents the square of the number, not a tensor index).

The covariant derivative of a tensor in coordinate direction  $a$  is denoted by the subscript ;  $a$ . The following are useful examples:

$$A_{;a} = \frac{\partial A}{\partial x^a}, \quad (\text{A.5})$$

$$B^a_{;b} = \frac{\partial B^a}{\partial x^b} + \Gamma^a_{cb} B^c, \quad (\text{A.6})$$

$$B_{a;b} = \frac{\partial B_a}{\partial x^b} - \Gamma^c_{ab} B_c, \quad (\text{A.7})$$

$$C^{ab}_{;c} = \frac{\partial C^{ab}}{\partial x^c} + \Gamma^a_{dc} C^{db} + \Gamma^b_{dc} C^{ad}, \quad (\text{A.8})$$

$$C^a_{b;c} = \frac{\partial C^a_b}{\partial x^c} + \Gamma^a_{dc} C^d_b - \Gamma^d_{bc} C^a_d, \quad (\text{A.9})$$

$$C_{ab;c} = \frac{\partial C_{ab}}{\partial x^c} - \Gamma^d_{ac} C_{db} - \Gamma^d_{bc} C_{ad}. \quad (\text{A.10})$$

The connection coefficients  $\Gamma^a_{bc}$ , used to evaluate covariant derivatives, are given by

$$\Gamma^a_{bc} = g^{ad} \Gamma_{dbc}, \quad \Gamma_{dbc} = \frac{1}{2} \left( \frac{\partial g_{db}}{\partial x^c} + \frac{\partial g_{dc}}{\partial x^b} - \frac{\partial g_{bc}}{\partial x^d} \right), \quad (\text{A.11})$$

and are symmetric on the last two indices ( $\Gamma^a_{bc} = \Gamma^a_{cb}$ ), due to the symmetry of the metric. Note that  $\Gamma^a_{bc}$  is not itself a tensor. The connection coefficients also satisfy the equation

$$\Gamma^a_{ba} = \frac{1}{g} \frac{\partial g}{\partial x^b} = \frac{\partial}{\partial x^b} \ln g, \quad (\text{A.12})$$

where  $g = \sqrt{|\det(g_{ab})|}$ .



## A.2 The Coordinate Invariant Fluid Equations

The density ( $\rho$ ), pressure ( $p$ ), and total energy density ( $e$ ) of a fluid are scalar fields and are invariant under coordinate transformations. The coordinate velocity ( $u^a$ ), momentum density ( $m_a = \rho u_a = \rho g_{ab} u^b$ ), mass flux ( $\rho u^a$ ), and total energy flux ( $[e + p]u^a$ ) are vector (first rank tensor) fields. The momentum flux ( $\rho u^a u_b + p \delta_b^a$ ) is a second rank tensor.

The coordinate velocity  $u^a = dx^a/dt$  is the rate of change of a fluid element coordinate  $x^a$  with time, and is generally not the same as the physical velocity  $v_a$ , which is the rate of change of distance along coordinate axis  $x^a$ . In an orthogonal coordinate system, where the coordinate axes are at right angles to each other, the metric  $g_{ab}$  is diagonal, with diagonal elements  $g_{aa} = h_a^2$ . In such a system the physical and coordinate velocities are related by  $v_a = h_a u^a$  (not summed).

Closing the system of equations requires auxiliary algebraic equations as well as the differential equations given below. The relationship between momentum density and velocity is one such equation:

$$u^a = g^{ab} u_b = g^{ab} m_b / \rho. \quad (\text{A.13})$$

Also useful is the velocity magnitude  $v$ , given by

$$v^2 \equiv u_a u^a = g_{ab} u^a u^b = v_1^2 + v_2^2 + v_3^2. \quad (\text{A.14})$$

The equation of state connects the pressure  $p$  to the thermal energy density  $\epsilon$  according to

$$p = (\gamma - 1)\epsilon, \quad \epsilon = e - \frac{1}{2}\rho v^2 = e - \frac{1}{2}m_a u^a. \quad (\text{A.15})$$

In simple perfect gas problems  $\gamma$  is the ratio of specific heats, and is a constant (equal to 5/3 for a monatomic gas). In more complicated problems (such as relativistic fluid dynamics)  $\gamma$  may be a function of the local fluid state, and is not the ratio of specific heats.

The equations given in this appendix include dissipative terms for use as artificial viscosity in finite difference calculations. The dissipation coefficient,  $\kappa$ , is taken to be nonzero only because the grid resolution used in the calculations is finite. To get the dissipation-free equations, simply set  $\kappa = 0$  throughout. The definition for  $\kappa$  is given in Chapter 4 and will not be repeated here.

The coordinate invariant fluid equations, with dissipation, are

$$\frac{\partial \rho}{\partial t} + (\rho u^a)_{;a} = (\kappa \rho^{;a})_{;a}, \quad (\text{A.16})$$

$$\frac{\partial e}{\partial t} + [(e + p)u^a]_{;a} = (\kappa e^{;a})_{;a}, \quad (\text{A.17})$$

$$\frac{\partial m_a}{\partial t} + (m_a u^b + p \delta_a^b)_{;b} = (\kappa m_a^{;b})_{;b}, \quad (\text{A.18})$$

in terms of covariant derivatives, or

$$\frac{\partial \rho}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^a} (g \rho u^a) = \frac{1}{g} \frac{\partial}{\partial x^a} \left( g \kappa g^{ab} \frac{\partial \rho}{\partial x^b} \right), \quad (\text{A.19})$$

$$\frac{\partial e}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^a} [g(e+p)u^a] = \frac{1}{g} \frac{\partial}{\partial x^a} \left( g\kappa g^{ab} \frac{\partial e}{\partial x^b} \right), \quad (\text{A.20})$$

$$\begin{aligned} \frac{\partial m_a}{\partial t} + \frac{1}{g} \frac{\partial}{\partial x^b} (gm_a u^b) + \frac{\partial p}{\partial x^a} + \frac{1}{2} \rho u_c u_d \frac{\partial g^{cd}}{\partial x^a} \\ = \frac{1}{g} \frac{\partial}{\partial x^c} \left[ gg^{bc} \kappa \left( \frac{\partial m_a}{\partial x^b} - \Gamma_{ab}^d m_d \right) \right] - \Gamma_{ac}^e \left[ g^{bc} \kappa \left( \frac{\partial m_e}{\partial x^b} - \Gamma_{eb}^d m_d \right) \right], \end{aligned} \quad (\text{A.21})$$

where  $g = \sqrt{|\det(g_{ab})|}$ .

The following sections give the fluid equations explicitly in rectangular, cylindrical, and spherical coordinates. It should be noted that the forms of the equations given are not exactly those obtained from the above calculations. Care has been taken to remove terms which cancel each other (especially when the terms individually become infinite, at singularities) and to cast the equations in a form well suited for finite difference calculations. *The direct translation of the tensor forms given above into finite difference forms leads to serious cancellation errors. One should always eliminate cancellations and singularities by hand to the greatest degree possible before resorting to numerical approximations.*

### A.3 Rectangular Coordinates

The coordinates are  $x^a = (x, y, z)$ . The metric and its inverse are

$$g_{ab} = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}, \quad g^{ab} = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}, \quad (\text{A.22})$$

and the metric factor  $g = 1$ . The contravariant (coordinate), covariant, and physical velocities are the same in this (and only this) coordinate system:

$$\begin{aligned} u^a &= (\dot{x}, \dot{y}, \dot{z}), \\ u_a &= (\dot{x}, \dot{y}, \dot{z}), \\ v_a &= (\dot{x}, \dot{y}, \dot{z}) = (u^x, u^y, u^z). \end{aligned} \quad (\text{A.23})$$

#### A.3.1 Connection Coefficients

All connection coefficients are zero:

$$\Gamma_{bc}^a = 0. \quad (\text{A.24})$$

### A.3.2 The Fluid Equations with Dissipation

Set  $\kappa = 0$  throughout for the inviscid equations.

#### Density

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u^x) + \frac{\partial}{\partial y}(\rho u^y) + \frac{\partial}{\partial z}(\rho u^z) \\ = \frac{\partial}{\partial x} \left( \kappa \frac{\partial \rho}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial \rho}{\partial y} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial \rho}{\partial z} \right), \end{aligned} \quad (\text{A.25})$$

#### Energy

$$\begin{aligned} \frac{\partial e}{\partial t} + \frac{\partial}{\partial x}[(e + p)u^x] + \frac{\partial}{\partial y}[(e + p)u^y] + \frac{\partial}{\partial z}[(e + p)u^z] \\ = \frac{\partial}{\partial x} \left( \kappa \frac{\partial e}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial e}{\partial y} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial e}{\partial z} \right), \end{aligned} \quad (\text{A.26})$$

#### $x$ momentum

$$\begin{aligned} \frac{\partial m_x}{\partial t} + \frac{\partial}{\partial x}(m_x u^x) + \frac{\partial}{\partial y}(m_x u^y) + \frac{\partial}{\partial z}(m_x u^z) + \frac{\partial p}{\partial x} \\ = \frac{\partial}{\partial x} \left( \kappa \frac{\partial m_x}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial m_x}{\partial y} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial m_x}{\partial z} \right) \end{aligned} \quad (\text{A.27})$$

#### $y$ momentum

$$\begin{aligned} \frac{\partial m_y}{\partial t} + \frac{\partial}{\partial x}(m_y u^x) + \frac{\partial}{\partial y}(m_y u^y) + \frac{\partial}{\partial z}(m_y u^z) + \frac{\partial p}{\partial y} \\ = \frac{\partial}{\partial x} \left( \kappa \frac{\partial m_y}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial m_y}{\partial y} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial m_y}{\partial z} \right) \end{aligned} \quad (\text{A.28})$$

#### $z$ momentum

$$\begin{aligned} \frac{\partial m_z}{\partial t} + \frac{\partial}{\partial x}(m_z u^x) + \frac{\partial}{\partial y}(m_z u^y) + \frac{\partial}{\partial z}(m_z u^z) + \frac{\partial p}{\partial z} \\ = \frac{\partial}{\partial x} \left( \kappa \frac{\partial m_z}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa \frac{\partial m_z}{\partial y} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial m_z}{\partial z} \right), \end{aligned} \quad (\text{A.29})$$

## A.4 Cylindrical Coordinates

The coordinates are  $x^a = (r, \phi, z)$ , and are related to rectangular coordinates by

$$\begin{aligned} x &= r \cos \phi, & r &= \sqrt{x^2 + y^2}, \\ y &= r \sin \phi, & \tan \phi &= y/x, \\ z &= z, & z &= z \end{aligned} \quad (\text{A.30})$$

The metric and its inverse are

$$g_{ab} = \begin{pmatrix} 1 & & \\ & r^2 & \\ & & 1 \end{pmatrix}, \quad g^{ab} = \begin{pmatrix} 1 & & \\ & r^{-2} & \\ & & 1 \end{pmatrix}, \quad (\text{A.31})$$

and the metric factor  $g = r$ . The contravariant (coordinate), covariant, and physical velocities are related by

$$\begin{aligned} u^a &= (\dot{r}, \dot{\phi}, \dot{z}), \\ u_a &= (\dot{r}, r^2 \dot{\phi}, \dot{z}), \\ v_a &= (\dot{r}, r \dot{\phi}, \dot{z}) = (u^r, r u^\phi, u^z). \end{aligned} \quad (\text{A.32})$$

#### A.4.1 Connection Coefficients

The connection coefficients are

$$\begin{aligned} \Gamma_{\phi\phi}^r &= -r, \\ \Gamma_{r\phi}^\phi &= \Gamma_{\phi r}^\phi = \frac{1}{r}. \end{aligned} \quad (\text{A.33})$$

All other  $\Gamma_{bc}^a = 0$ .

#### A.4.2 The Fluid Equations with Dissipation

Set  $\kappa = 0$  throughout for the inviscid equations.

**Density**

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r \rho u^r) + \frac{\partial}{\partial \phi} (\rho u^\phi) + \frac{\partial}{\partial z} (\rho u^z) \\ = \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa \frac{\partial \rho}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \phi} \left( \kappa \frac{\partial \rho}{\partial \phi} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial \rho}{\partial z} \right), \end{aligned} \quad (\text{A.34})$$

**Energy**

$$\begin{aligned} \frac{\partial e}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} [r(e+p)u^r] + \frac{\partial}{\partial \phi} [(e+p)u^\phi] + \frac{\partial}{\partial z} [(e+p)u^z] \\ = \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa \frac{\partial e}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \phi} \left( \kappa \frac{\partial e}{\partial \phi} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial e}{\partial z} \right), \end{aligned} \quad (\text{A.35})$$

**$r$  momentum**

$$\frac{\partial m_r}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r m_r u^r) + \frac{\partial}{\partial \phi} (m_r u^\phi) + \frac{\partial}{\partial z} (m_r u^z) + \frac{\partial p}{\partial r} - r \rho u^{\phi 2}$$

$$= \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa \frac{\partial m_r}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \phi} \left[ \kappa \left( \frac{\partial m_r}{\partial \phi} - \frac{m_\phi}{r} \right) \right] + \frac{\partial}{\partial z} \left( \kappa \frac{\partial m_r}{\partial z} \right) - \frac{1}{r^3} \kappa \left( \frac{\partial m_\phi}{\partial \phi} + r m_r \right), \quad (\text{A.36})$$

$\phi$  momentum

$$\begin{aligned} \frac{\partial m_\phi}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r m_\phi u^r) + \frac{\partial}{\partial \phi} (m_\phi u^\phi) + \frac{\partial}{\partial z} (m_\phi u^z) + \frac{\partial p}{\partial \phi} \\ = \frac{1}{r} \frac{\partial}{\partial r} \left[ r \kappa \left( \frac{\partial m_\phi}{\partial r} - \frac{m_\phi}{r} \right) \right] + \frac{1}{r^2} \frac{\partial}{\partial \phi} \left[ \kappa \left( \frac{\partial m_\phi}{\partial \phi} + r m_r \right) \right] \\ + \frac{\partial}{\partial z} \left( \kappa \frac{\partial m_\phi}{\partial z} \right) + \frac{1}{r} \kappa \left( \frac{\partial m_r}{\partial \phi} - \frac{\partial m_\phi}{\partial r} \right), \end{aligned} \quad (\text{A.37})$$

$z$  momentum

$$\begin{aligned} \frac{\partial m_z}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r m_z u^r) + \frac{\partial}{\partial \phi} (m_z u^\phi) + \frac{\partial}{\partial z} (m_z u^z) + \frac{\partial p}{\partial z} \\ = \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa \frac{\partial m_z}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \phi} \left( \kappa \frac{\partial m_z}{\partial \phi} \right) + \frac{\partial}{\partial z} \left( \kappa \frac{\partial m_z}{\partial z} \right), \end{aligned} \quad (\text{A.38})$$

## A.5 Spherical Coordinates

The coordinates are  $x^a = (r, \theta, \phi)$ , and are related to rectangular coordinates by

$$\begin{aligned} x &= r \sin \theta \cos \phi, & r &= \sqrt{x^2 + y^2 + z^2}, \\ y &= r \sin \theta \sin \phi, & \tan \theta &= \frac{\sqrt{x^2 + y^2}}{z} \\ z &= r \cos \theta, & \tan \phi &= y/x \end{aligned} \quad (\text{A.39})$$

The metric and its inverse are

$$g_{ab} = \begin{pmatrix} 1 & & \\ & r^2 & \\ & & r^2 \sin^2 \theta \end{pmatrix}, \quad g^{ab} = \begin{pmatrix} 1 & & \\ & r^{-2} & \\ & & r^{-2} \sin^{-2} \theta \end{pmatrix}, \quad (\text{A.40})$$

and the metric factor  $g = r^2 \sin \theta$ . The contravariant (coordinate), covariant, and physical velocities are related by

$$\begin{aligned} u^a &= (\dot{r}, \dot{\theta}, \dot{\phi}), \\ u_a &= (\dot{r}, r^2 \dot{\theta}, r^2 \sin^2 \theta \dot{\phi}), \\ v_a &= (\dot{r}, r \dot{\theta}, r \sin \theta \dot{\phi}) = (u^r, r u^\theta, r \sin \theta u^\phi). \end{aligned} \quad (\text{A.41})$$

### A.5.1 Connection Coefficients

The connection coefficients are

$$\begin{aligned}\Gamma_{\theta\theta}^r &= -r, & \Gamma_{\phi\phi}^r &= -r \sin^2 \theta, \\ \Gamma_{r\theta}^\theta &= \Gamma_{\theta r}^\theta = \frac{1}{r}, & \Gamma_{\phi\phi}^\theta &= -\sin \theta \cos \theta, \\ \Gamma_{r\phi}^\phi &= \Gamma_{\phi r}^\phi = \frac{1}{r}, & \Gamma_{\theta\phi}^\phi &= \Gamma_{\phi\theta}^\phi = \cot \theta.\end{aligned}\tag{A.42}$$

All other  $\Gamma_{bc}^a = 0$ .

### A.5.2 The Fluid Equations with Dissipation

Set  $\kappa = 0$  throughout for the inviscid equations.

**Density**

$$\begin{aligned}\frac{\partial \rho}{\partial t} &+ \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho u^r) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \rho u^\theta) + \frac{\partial}{\partial \phi} (\rho u^\phi) \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa \frac{\partial \rho}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \kappa \frac{\partial \rho}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \phi} \left( \kappa \frac{\partial \rho}{\partial \phi} \right),\end{aligned}\tag{A.43}$$

**Energy**

$$\begin{aligned}\frac{\partial e}{\partial t} &+ \frac{1}{r^2} \frac{\partial}{\partial r} [r^2 (e + p) u^r] + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} [\sin \theta (e + p) u^\theta] + \frac{\partial}{\partial \phi} [(e + p) u^\phi] \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa \frac{\partial e}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \kappa \frac{\partial e}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \phi} \left( \kappa \frac{\partial e}{\partial \phi} \right),\end{aligned}\tag{A.44}$$

**$r$  momentum**

$$\begin{aligned}\frac{\partial m_r}{\partial t} &+ \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 m_r u^r) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (\sin \theta m_r u^\theta) + \frac{\partial}{\partial \phi} (m_r u^\phi) \\ &+ \frac{\partial p}{\partial r} - r \rho (u^{\theta 2} + \sin^2 \theta u^{\phi 2}) \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa \frac{\partial m_r}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left[ \sin \theta \kappa \left( \frac{\partial m_r}{\partial \theta} - \frac{m_\theta}{r} \right) \right] \\ &+ \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \phi} \left[ \kappa \left( \frac{\partial m_r}{\partial \phi} - \frac{m_\phi}{r} \right) \right] \\ &- \frac{1}{r^3} \kappa \left( \frac{\partial m_\theta}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial m_\phi}{\partial \phi} + 2r m_r + \cot \theta m_\theta \right),\end{aligned}\tag{A.45}$$

**$\theta$  momentum**

$$\frac{\partial m_\theta}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 m_\theta u^r) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (\sin \theta m_\theta u^\theta) + \frac{\partial}{\partial \phi} (m_\theta u^\phi)$$

$$\begin{aligned}
& + \frac{\partial p}{\partial \theta} - r^2 \sin \theta \cos \theta \rho u^{\phi^2} \\
& = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \kappa \left( \frac{\partial m_\theta}{\partial r} - \frac{m_\theta}{r} \right) \right] + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \kappa \frac{\partial m_\theta}{\partial \theta} \right) \\
& \quad + \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \phi} \left[ \kappa \left( \frac{\partial m_\theta}{\partial \phi} - \cot \theta m_\phi \right) \right] \\
& \quad + \frac{1}{r} \kappa \left( \frac{\partial m_r}{\partial \theta} - \frac{\partial m_\theta}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} (\kappa m_r) - \frac{\cot \theta}{r^2} \kappa \left( \frac{1}{\sin^2 \theta} \frac{\partial m_\phi}{\partial \phi} + \cot \theta m_\theta \right),
\end{aligned} \tag{A.46}$$

$\phi$  momentum

$$\begin{aligned}
& \frac{\partial m_\phi}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 m_\phi u^r) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (\sin \theta m_\phi u^\theta) + \frac{\partial}{\partial \phi} (m_\phi u^\phi) + \frac{\partial p}{\partial \phi} \\
& = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \kappa \left( \frac{\partial m_\phi}{\partial r} - \frac{m_\phi}{r} \right) \right] + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left[ \kappa \left( \sin \theta \frac{\partial m_\phi}{\partial \theta} - \cos \theta m_\theta \right) \right] \\
& \quad + \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \phi} \left[ \kappa \left( \frac{\partial m_\phi}{\partial \phi} + r \sin^2 \theta m_r + \sin \theta \cos \theta m_\theta \right) \right] \\
& \quad + \frac{1}{r} \kappa \left( \frac{\partial m_r}{\partial \phi} - \frac{\partial m_\phi}{\partial r} \right) + \frac{\cot \theta}{r^2} \kappa \left( \frac{\partial m_\theta}{\partial \phi} - \frac{\partial m_\phi}{\partial \theta} \right).
\end{aligned} \tag{A.47}$$

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16. Abstract  These lecture notes cover the basic principles of computational fluid dynamics (CFD). They are oriented more toward practical applications than theory, and are intended to serve as a unified source for basic material in the CFD field as well as an introduction to more specialized topics in artificial viscosity and boundary conditions. Each chapter in the text is associated with a videotaped lecture; the videotapes may be obtained from the author.  Chapter 1 of the notes describes the basic properties of conservation laws, wave equations, and shock waves. The duality of the conservation law and wave representations is investigated, and shock waves are examined in some detail. Chapter 2 introduces finite difference techniques for the solution of wave equations and conservation laws. Chapter 3 presents stability analysis for finite difference approximations. Chapter 4 provides a consistent description of artificial viscosity methods. Finally, Chapter 5 treats the problem of nonreflecting boundary conditions.					
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